OPTIMIZATION OF COMPOSITE PROCESSES AND VARIATIONAL TECHNIQUES

by

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I. INTRODUCTION

For the past ten years the mathematical techniques of optimization have been rapidly improving and finding wide applications in various fields. The purpose of optimization is to design a process in such a way that under certain restrictions the maximum profit may be obtained. Among many techniques for solving the problems, the calculus of variations, the method of gradients, dynamic programming, and the maximum principle are generally regarded as the most powerful ones. Each of these methods has comparative advantages over one another, depending on the problem to be solved.

Theories of the calculus of variations and the method of gradients were well and fully developed long before. In 1957 Bellman presented the method of dynamic programming (1) which is very useful in the solution of multistage decision processes. In 1956 Pontryagin proposed the maximum principle (2) for treating the time-optimal continuous processes. The first attempt to extend it to the optimization of stagewise processes was made by Rozonoer (3) in 1959. Chang (4) and Katz (5) independently presented the discrete version of the maximum principle in 1960. The generalization of the discrete version to treat different complex processes was made by Fan and Wang (6) and Aris and Denn (7) recently.

Every chemical plant consists of many interconnected process units, each of which is either discrete, continuous, or a combination of both. The discrete processes can generally be described by a system of difference equations and the continuous processes by a system of differential equations. A process which is composed of both discrete and continuous processes is referred to as a composite process.

As a process becomes complicated, the number of operating variables increases and the techniques used to treat the problems are therefore restricted. The generalization of the maximum principle to treat complex continuous processes has been presented by Fan and Wang (8). The main purpose of the present thesis is to extend the maximum principle to treat topologically complex composite processes and derive working algorithms that overcome the difficulties which the other methods may encounter.

The underlying idea of the maximum principle is to transform the original system of equations to a new system of equivalent equations such that the new system is easier to handle and clearer to visualize. The relationships between this transformation, the calculus of variations, and dynamic programming are also discussed in detail.

II. THE MAXIMUM PRINCIPLE

The continuous maximum principle was first developed by the Russian mathematician Pontryagin. His original version was essentially used to treat control problems. In this chapter the procedures for solving problems and the basic algorithms for simple continuous and discrete processes are derived.

Algorithms for Simple Continuous Processes

A simple continuous process, shown schematically in Figure 1, can be described by differential equations of the form

$$\dot{x}_i(t) = \frac{dx_i}{dt} = f_i(x_1(t), x_2(t), \ldots, x_s(t); \theta_1(t), \theta_2(t), \ldots, \theta_r(t))$$

$$t_0 \leq t \leq T, \qquad i = 1, 2, \ldots, s$$

$$x(t) = \alpha_i, \qquad i = 1, 2, \ldots, s$$

or, in vector form,

$$\dot{x}(t) = \frac{dx}{dt} = f(x(t); \theta(t)), \qquad t_0 \leq t \leq T$$
$$x(t_0) = \alpha \tag{1}$$

where $x(t)$ is an s-dimensional vector function representing the state of the process at time t, $\theta(t)$ is an r-dimensional vector function representing the decision (or control) at time t, and α, a constant vector, is the initial value of the state vector $x(t)$.

A typical optimization problem associated with such a process is to find a piecewise continuous decision vector function, $\theta(t)$, subject to the constraints

$$\psi\left[\theta_1(t), \theta_2(t), \ldots, \theta_r(t)\right] \leq 0, \qquad i = 1, 2, \ldots, m \tag{2}$$

which makes a function of the final values of the state

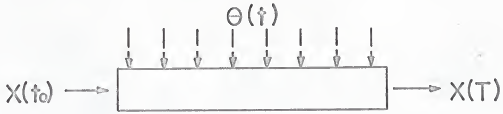


Fig. I. A simple process.

$$S = \sum_{i=1}^{s} c_i x_i(T) , \qquad c_i = \text{constant} \tag{3}$$

an extremum when the initial condition $x(t_0) = \alpha$ is given. The function $S = \sum_{i=1}^{s} c_i x_i(T)$, which is to be maximized (or minimized), is called the objective function of the process. The decision vector so chosen is called an optimal decision vector function or simply an optimal decision and is denoted by $\bar{\theta}(t)$.

The procedure for solving the problem is to introduce an s-dimensional adjoint vector $z(t)$ and a Hamiltonian function H which satisfy the following relations:

$$H(z(t), x(t), \theta(t)) = \sum_{i=1}^{s} z_i f_i(x(t); \theta(t)). \tag{4}$$

$$\frac{dz_i}{dt} = - \frac{\partial H}{\partial x_i} , \qquad i = 1, 2, \ldots, s. \tag{5}$$

$$z_i(T) = c_i , \qquad i = 1, 2, \ldots, s. \tag{6}$$

It will be shown that if the optimal decision vector $\theta(t)$ is interior to the set of admissible decisions $\theta(t)$, given by Equation (2), a necessary condition for S to be an extremum with respect to $\theta(t)$ is

$$\frac{\partial H}{\partial \theta} = 0. \tag{7}$$

If $\theta(t)$ is constrained, the optimal decision is determined either by solving Equation (7) for $\theta(t)$ or by searching the boundary of the set.

Assume that the function $f(x(t); \theta(t))$ is continuous in its arguments and the first partial derivatives exist and are piecewise continuous in their arguments. Let $\bar{x}(t)$ be the optimal state vector of the process corresponding to the optimal decision $\bar{\theta}(t)$, then

$$\frac{d\bar{x}}{dt} = f(\bar{x}(t);\ \theta(t)). \tag{8}$$

A small perturbation of $\theta(t)$ from $\bar{\theta}(t)$ can be represented by

$$\theta(t,\epsilon) = \bar{\theta}(t) + \epsilon\varphi(t) + O(\epsilon^2), \tag{9}$$

and the resulting perturbation of $x(t)$ is then

$$x(t,\epsilon) = \bar{x}(t) + \epsilon y(t) + O(\epsilon^2). \tag{10}$$

where ϵ is a small number, φ and y are bounded functions of t, and $O(\epsilon^2)$ denotes the ϵ^2 term and those of order higher than ϵ^2.

A variational equation can be obtained from Equations (1) and (8) as

$$\epsilon \frac{dy_i}{dt} = f_i(x;\theta) - f_i(\bar{x};\bar{\theta}) + O(\epsilon^2)\ , \qquad i = 1, 2, \ldots, s. \tag{11}$$

Expanding Equation (11) in a Taylor series around $(\bar{x}(t);\bar{\theta}(t))$, one obtains

$$\epsilon \frac{dy_i}{dt} = \sum_{j=1}^{s} \epsilon y_j \frac{\partial f_i(x;\theta)}{\partial x_j} + \sum_{j=1}^{r} \epsilon\varphi_j \frac{\partial f_i(x;\theta)}{\partial \theta_j} + O(\epsilon^2)\ , \tag{12}$$

$$i = 1, 2, \ldots, s$$

where the partial derivatives are evaluated at $(\bar{x}(t);\bar{\theta}(t))$.

If Equations (5) and (12) are substituted into the expression

$$\frac{d}{dt}\sum_{i=1}^{s} \epsilon y_i z_i = \sum_{i=1}^{s} \epsilon z_i \frac{dy_i}{dt} + \sum_{i=1}^{s} \epsilon y_i \frac{dz_i}{dt} \tag{13}$$

one obtains

$$\frac{d}{dt}\sum_{i=1}^{s} \epsilon y_i z_i = \sum_{i=1}^{s} z_i \left[\sum_{j=1}^{s} \epsilon y_j \frac{\partial f_i}{\partial x_j} + \sum_{j=1}^{r} \epsilon\varphi_j \frac{\partial f_i}{\partial \theta_j} + O(\epsilon^2)\right]$$

$$+ \sum_{i=1}^{s} \epsilon y_i \left(-\frac{\partial H}{\partial x_i}\right)$$

$$= \sum_{i=1}^{s}\sum_{j=1}^{r} z_i \frac{\partial f_i}{\partial \theta_j}\epsilon\varphi_j + O(\epsilon^2). \tag{14}$$

Considering the linear terms in Equation (14) and integrating from $t = t_0$

to $t = T$ yields

$$\sum_{i=1}^{s} \epsilon \left[y_i(T) z_i(T) - y_i(t_0) z_i(t_0) \right] = \int_{t_0}^{T} \sum_{i=1}^{s} \sum_{j=1}^{r} z_i \frac{\partial f_i}{\partial \theta_j} \epsilon\varphi_j \, dt. \tag{15}$$

Since the initial value of $x(t)$ is given and fixed, we have

$$\epsilon y_i(t_0) = 0 , \qquad i = 1, 2, \ldots, s. \tag{16}$$

Substitution of Equations (6) and (16) into Equation (15) and use of the definition of the Hamiltonian gives

$$\sum_{i=1}^{s} \epsilon c_i y_i(T) = \int_{0}^{T} \sum_{j=1}^{r} \frac{\partial H}{\partial \theta_j} \epsilon\varphi_j \, dt. \tag{17}$$

Suppose the objective function has a maximum. The quantity on the left hand side of Equation (17) is the variation of the objective function S, which must be zero along the optimal trajectory for free variations (unconstrained variation) and be negative for variations at the boundary of the constraints, that is,

$$\sum_{i=1}^{s} \epsilon c_i y_i(T) \leq 0 , \tag{18}$$

Thus from Equations (17) and (18) we conclude that for arbitrary $\epsilon\varphi$ the necessary conditions for S to be a maximum are

$$\frac{\partial H}{\partial \theta_j} = 0 \qquad \text{at } \theta_j(t) = \bar{\theta}_j(t) , \quad t_0 \leq t \leq T , \quad j = 1, 2, \ldots, r. \tag{19}$$

when $\bar{\theta}_j(t)$ lies in the interior of the region of $\theta(t)$, or

$$H = \max \quad \text{at } \theta_j(t) = \bar{\theta}_j(t) , \quad t_0 \leq t \leq T , \quad j = 1, 2, \ldots, r \tag{20}$$

when $\bar{\theta}_j(t)$ lies at the boundary of the constraints. If the objective function S has a minimum, then reversing the inequality signs in the above derivations will give H = min. in Equation (20).

Algorithms for Simple Discrete Processes

A simple discrete process, shown schematically in Figure 2, can be described by difference equations of the form

$$x_i^n = T^n\,(x_1^{n-1}, x_2^{n-1}, \ldots, x_s^{n-1}\ ;\ \theta_1^n, \theta_2^n, \ldots, \theta_r^n), \quad i = 1, 2, \ldots, s$$

$$x_i^0 = \alpha_i.$$

or, in vector form,

$$x^n = T^n\,(x^{n-1};\ \theta^n). \qquad x^0 = \alpha. \tag{21}$$

where x^n is an s-dimensional vector function representing the state of the process at the nth stage, θ^n is an r-dimensional vector function representing the decision (or control) at the nth stage, and α is a given constant vector.

The adjoint vectors and the Hamiltonian function are defined as

$$H^n(z^n, x^n, \theta^n) = \sum_{i=1}^{s} z_i^n T_i^n(x^{n-1};\ \theta^n)\ , \qquad n = 1, 2, \ldots, N. \tag{22}$$

$$z_i^{n-1} = \frac{\partial H^n}{\partial x_i^{n-1}} = \sum_{j=1}^{s} z_j^n \frac{\partial T_j^n(x^{n-1};\theta^n)}{\partial x_i^{n-1}}\ , \qquad \begin{matrix} i = 1, 2, \ldots, s \\ n = 1, 2, \ldots, N. \end{matrix} \tag{23}$$

$$z_i^N = c_i\ , \qquad i = 1, 2, \ldots, s. \tag{24}$$

The objective function is generally of the form

$$S = \sum_{i=1}^{s} c_i x_i^N\ . \tag{25}$$

The necessary conditions for S to be an extremum are found from

$$\frac{\partial H^n}{\partial \theta^n} = 0\ , \qquad n = 1, 2, \ldots, N. \tag{26}$$

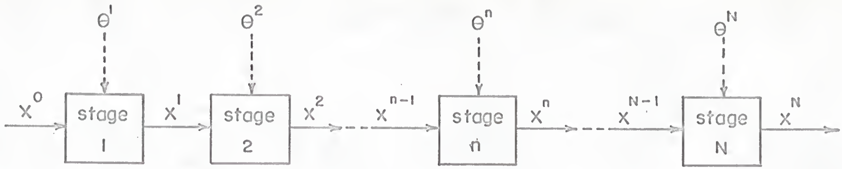


Fig. 2. A simple discrete process.

or by searching the boundary of the set of $\theta(t)$.

The proof is parallel to that of the continuous case. Let $\bar{\theta}^n$ be the optimal decision and $\bar{x}^n$ the corresponding state vector. Then we have

$$\theta^n = \bar{\theta}^n + \epsilon\varphi^n + O(\epsilon^2) , \qquad n = 1, 2, \ldots, N. \tag{27}$$

$$x^n = \bar{x}^n + \epsilon y^n + O(\epsilon^2) , \qquad n = 1, 2, \ldots, N. \tag{28}$$

Combining Equation (21) and (28) gives

$$\begin{aligned} \epsilon y^n &= T^n(x^{n-1};\theta^n) - T^n(\bar{x}^{n-1};\bar{\theta}^n) + O(\epsilon^2) , \\ & i = 1, 2, \ldots, s; \quad n = 1, 2, \ldots, N. \end{aligned} \tag{29}$$

Expanding Equation (29) in a Taylor series around

$$\epsilon y_i^n = \sum_{j=1}^{s} \epsilon y_j^{n-1} \frac{\partial T_i^n(x^{n-1};\theta^n)}{\partial x_j^{n-1}} + \sum_{j=1}^{r} \epsilon\varphi_j^n \frac{\partial T_i^n(x^{n-1};\theta^n)}{\partial \theta_j^n} + O(\epsilon^2) ,$$

$$i = 1, 2, \ldots, s; \quad n = 1, 2, \ldots, N$$

where the partial derivatives are evaluated at $(\bar{x}^{n-1};\bar{\theta}^n)$. Multiplying Equation (30) by z_i^n, summing on n from n = 1 to n = N and on i from i = 1 to i = s, and employing Equations (23) and (22) yield

$$\sum_{i=1}^{s} \epsilon \left[y_i^N z_i^N - y_i^0 z_i^0\right] = \sum_{n=1}^{N} \sum_{i=1}^{s} \sum_{j=1}^{r} z_i^n \frac{\partial T_i^n(x^{n-1};\theta^n)}{\partial \theta_j^n} \epsilon\varphi_j^n + O(\epsilon^2). \tag{31}$$

Since the initial value of x^n is given and fixed, we have

$$\epsilon y_i^0 = 0 , \qquad i = 1, 2, \ldots, s. \tag{32}$$

Considering the linear terms in Equation (31) and using the definition of the Hamiltonian and Equations (24) and (32), one obtains

$$\sum_{i=1}^{s} \epsilon c_i y_i^N = \sum_{n=1}^{N} \sum_{j=1}^{r} \frac{\partial H^n}{\partial \theta_j} \epsilon\varphi_j^n . \tag{33}$$

Suppose that S has a maximum. The left hand side of Equation (33) is the variation of the objective function and must be zero for free variations and be negative for variations at the boundary of the set of θ^n, that is

$$\sum_{i=1}^{s} \epsilon c_i y_i^N \leq 0 \ . \tag{34}$$

Thus from Equations (33) and (34) we conclude that for arbitrary $\epsilon\varphi^n$ the necessary conditions for S to be an extremum are

$$\frac{\partial H^n}{\partial \theta^n} = 0 \qquad \text{at} \qquad \theta^n = \bar{\theta}^n \ , \quad n = 1, 2, \ldots, N$$

when $\bar{\theta}^n$ lies in the interior of the region of θ^n, or

$$H = \max \qquad \text{at} \qquad \theta^n = \bar{\theta}^n \ , \quad n = 1, 2, \ldots, N \tag{36}$$

when $\bar{\theta}^n$ lies at the boundary of the constraints.

It is to be noted that the necessary conditions for S to be a maximum (or minimum) in the continuous case can be strengthened so that if S is maximum (or minimum), then H is a maximum (or minimum). However, in the discrete case there is no such analog. The strengthened condition will be proved later.

III. OPTIMIZATION OF COMPOSITE PROCESSES AND APPLICATIONS

The optimization of complex discrete processes and complex continuous processes has already been treated extensively (6, 8). Many processes in practice, however, are encountered in the combined form. For convenience, such a complex process is called a composite process. In this section a general method of obtaining directly the optimal policy for a composite process, without decomposing it into subprocesses, is presented.

Statement and Derivation of the Algorithm

The algorithm is applicable to a composite process consisting of three basic types as shown in Figures 3, 4, and 5.

In a simple continuous process contained in a composite process, the change of the state can be described by the following performance equations

$$\frac{dx_i}{dt} = f_i(x_1(t), x_2(t), \ldots, x_s(t); \theta_1(t), \ldots, \theta_r(t)), \quad t_0 \leq t \leq T$$

$$i = 1, 2, \ldots, s$$

or, in vector form,

$$\frac{dx}{dt} = f(x(t); \theta(t)) \ . \tag{1}$$

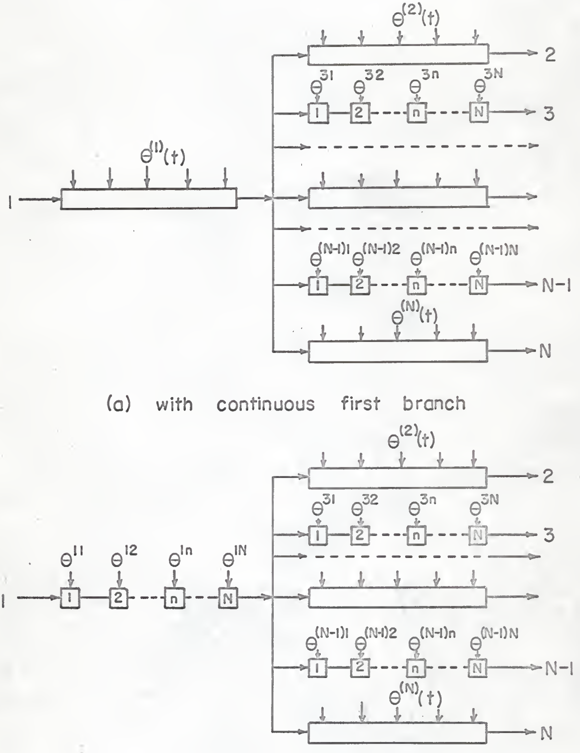
For a simple discrete process contained in a composite process the performance equations are

$$x_i^n = T^n(x_1^{n-1}, x_2^{n-1}, \ldots, x_s^{n-1}; \theta_1^n, \theta_2^n, \ldots, \theta_r^n) , \quad i = 1, 2, \ldots, s$$

or, in vector form,

$$x^n = T^n(x^{n-1}; \theta^n). \tag{2}$$

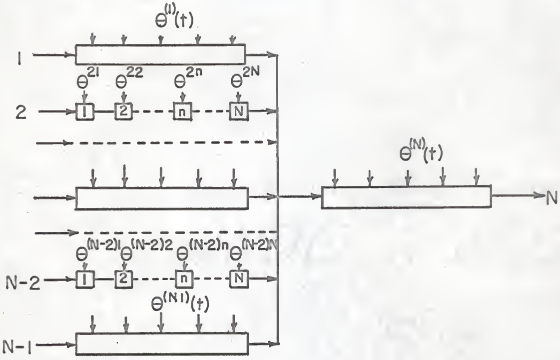
All of the composite processes are composed of several inter-connected branches. The point where two or more branches connect is called a junction



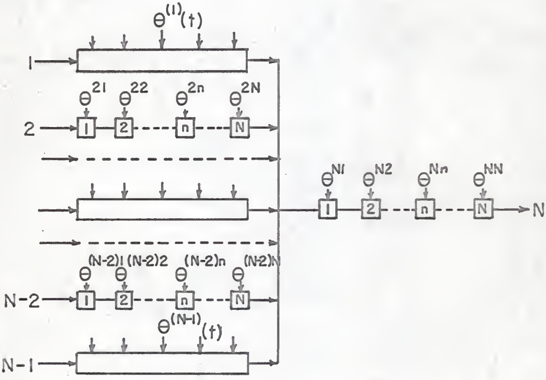
(a) with continuous first branch

(b) with discrete first branch

Fig. 3. Separating points in a composite process.



(a) with continuous last branch



(b) with discrete last branch

Fig. 4 Combining points in a composite process.

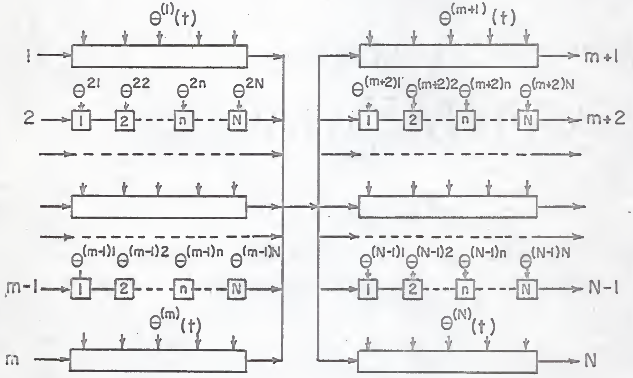


Fig. 5 A crossing point in a composite process.

point. There are, as shown in Figures 3, 4 and 5, three basic types of junction points (6, 8):

(a) A separating point is a point where one branch of the path splits into several branches.

(b) A combining point is a point where several branches combine into one single branch.

(c) A crossing point is a point where several branches combine together and then split again into several branches.

The relationships between the state vectors of different branches at the junction points are described by the following junction equations. They are as follows:

(1) Separating points

a. If the first branch (entering stream) is continuous (see Figure 3a)

$$x^{(k)}(0) \quad \text{or} \quad x^{k0} = g^{(k)}(x^{(1)}(T_1)), \quad k = 2, \ldots, N. \tag{3}*$$

b. If the first branch (entering stream) is discrete (see Figure 3b)

$$x^{(k)}(0) \quad \text{or} \quad x^{k0} = g^{(k)}(x^{1N}), \quad k = 2, \ldots, N. \tag{4}$$

(2) Combining points (see Figure 4)

$$x^{(N)}(0) \quad \text{or} \quad x^{N0} = g^{(N)}(x^{1N}, x^{2N}, \ldots, x^{d'N}, x^{(d'+1)}(T_{d'+1}), \ldots, x^{(N-1)}(T_{N-1})). \tag{5}$$

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* The nth stage in the kth discrete branch is denoted kn, and the kth continuous branch by (k). T_k is the length of the kth continuous branch.

c' and d' denote the number of continuous branches and the number of discrete branches entering a junction point respectively. Similarly c" and d" denote the number of continuous and discrete branches leaving the junction point respectively. The total number of the continuous branches is represented by c and that of the discrete branches by d.

(3) Crossing points (see Figure 5)

$$x^{(k)}(0) \quad \text{or} \quad x^{k0} = g^{(k)}(x^{1N}, x^{2N}, \ldots, x^{d'N}, x^{(d'+1)}(T_{d'+1}), \ldots, x^{(m)}(T_m)) , \tag{6}$$

$$k = m+1, m+2, \ldots, N.$$

The optimization problem under consideration may be stated as follows: Given all the performance equations, junction equations, lengths, number of stages and initial states of a composite process consisting of a path with N branches, b initial points, and e final points, find the optimal decision vector function of each continuous branch and the optimal decision vector at each stage in each discrete branch, so as to maximize a certain linear function of the final states of the process, the objective function,

$$S = \sum_{c''} \sum_{i=1}^{s^{(c'')}} c_i^{(c'')} x_i^{(c'')}(T_{c''}) + \sum_{d''} \sum_{i=1}^{s^{(d'')}} c_i^{d''N} x_i^{d''N} .$$

where c_i are constants; the superscripts c" and d" denote the labels of continuous and discrete branches respectively; $\sum_{c''}$ and $\sum_{d''}$ indicate the summation over all continuous and discrete branches with end points respectively. Similarly, $\sum_{c'}$ and $\sum_{d'}$ are used to denote the summation over all continuous and discrete branches with initial points respectively and $\sum_{c}$ and $\sum_{d}$ to denote the summation over all the continuous and discrete branches respectively.

To find the optimal decision vectors, adjoint vectors and Hamiltonian

functions satisfying the following relationships are introduced as follows:

(1) For each of the continuous branches

$$H^{(k)}(x,z,\theta) = \sum_{i=1}^{s^{(k)}} z_i^{(k)} f_i^{(k)}(x_1^{(k)},\ldots,x_{s^{(k)}}^{(k)};\ \theta_1^{(k)},\ldots,\ \theta_r^{(k)}). \quad (7)$$

$$\frac{dz_i^{(k)}}{dt} = -\frac{\partial H^{(k)}}{\partial x_i^{(k)}}, \qquad i = 1,\ 2,\ldots\ldots,\ s^{(k)} \quad (8)$$

(2) For each of the discrete branches

$$H^{kn} = \sum_{i=1}^{s} z_i^{kn}\, T_i^{kn}\,(x_1^{k(n-1)},\ldots,\ x_{s^{(k)}}^{k(n-1)};\ \theta_1^{kn},\ \theta_2^{kn},\ldots,\ \theta_r^{kn}). \quad (9)$$

$$z_i^{k(n-1)} = \frac{\partial H^{kn}}{\partial x_i^{k(n-1)}}, \qquad i = 1,\ 2,\ldots,\ s^{(k)}. \quad (10)$$

The values of the components of the adjoint vectors at the final points of the entering streams of each branch satisfy the following relations:

(a) Separating points

i) If the first branch is continuous

$$z_i^{(1)}(T_1) = \sum_{c''} \sum_{j=1}^{s^{(c'')}} \frac{\partial g_j^{(c'')}}{\partial x_i^{(1)}}\, z_j^{(c'')}(0) + \sum_{d''} \sum_{j=1}^{s^{(d'')}} \frac{\partial g_j^{(d'')}}{\partial x_i^{(1)}}\, z_j^{d''0}, \quad (11)$$

$$i = 1,\ 2,\ldots,\ s^{(1)}.$$

ii) If the first branch is discrete

$$z_i^{1N} = \sum_{c''} \sum_{j=1}^{s^{(c'')}} \frac{\partial g_j^{(c'')}}{\partial x_i^{1N}}\, z_j^{(c'')}(0) + \sum_{d''} \sum_{j=1}^{s^{(d'')}} \frac{\partial g_j^{(d'')}}{\partial x_i^{1N}}\, z_j^{d''0}, \quad (12)$$

$$i = 1,\ 2,\ldots,\ s^{(1)}.$$

(b) Combining points

For the case in which branch N is either continuous or discrete one has the following relations:

i) For the continuous entering branches

$$z_i^{(k)}(T_k) = \sum_{j=1}^{s^{(N)}} \frac{\partial g_j^{(N)}}{\partial x_i^{(k)}} z_j^{(N)}(0) \ , \qquad \begin{array}{l} i = 1, 2, \ldots, s^{(k)} \\ k = 1, 2, \ldots, c'. \end{array} \tag{13}$$

ii) For the discrete entering branches

$$z_i^{kN} = \sum_{j=1}^{s^{(N)}} \frac{\partial g_j^{(N)}}{\partial x_i^{kN}} z_j^{(N)}(0), \qquad \begin{array}{l} i = 1, 2, \ldots, s^{(k)} \\ k = c'+1, c'+2, \ldots, N-1. \end{array} \tag{14}^*$$

(c) Crossing points

i) For the continuous entering branches

$$z_i^{(k)}(T_k) = \sum_{c''} \sum_{j=1}^{s^{(c'')}} \frac{\partial g_j^{(c'')}}{\partial x_i^{(k)}} z_j^{(c'')}(0) + \sum_{d''} \sum_{j=1}^{s^{(d'')}} \frac{\partial g_j^{(d'')}}{\partial x_i^{(k)}} z_j^{d''0} \ , \qquad \begin{array}{l} i = 1, 2, \ldots, z^{(k)} \\ k = 1, \ldots, c'. \end{array} \tag{15}$$

ii) For the discrete entering branches

$$z_i^{kN} = \sum_{c''} \sum_{j=1}^{s^{(c'')}} \frac{\partial g_j^{(c'')}}{\partial x_i^{kN}} z_j^{(c'')}(0) + \sum_{d''} \sum_{j=1}^{s^{(d'')}} \frac{\partial g_j^{(d'')}}{\partial x_i^{kN}} z_j^{d''0}, \qquad \begin{array}{l} i=1,2,\ldots, s^{(k)} \\ k=c'+1, \ldots, m. \end{array} \tag{16}$$

(d) Final points

$$\begin{array}{ll} z_i^{(c'')}(T_{c''}) = c_i^{(c'')} \ , & i = 1, 2, \ldots, s^{(c'')} \\ z_i^{d''N} = c_i^{d''N} \ , & i = 1, 2, \ldots, s^{(d'')}. \end{array} \tag{17}$$

The optimal decisions for every continuous branch are then determined from the following necessary conditions:

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* Equations (13) and (14) are written for the case branch N is continuous. If it is discrete, $z_i^{(N)}(0)$ in the equations is replaced by z_i^{N0}.

$$\frac{\partial H^{(k)}}{\partial \theta^{(k)}} = 0 \quad \text{or} \quad H^{(k)} = \text{maximum at every point } t, \quad t_0 \leq t \leq T_k \qquad (18)^*$$

and for each discrete branch

$$\begin{aligned} & H^{kn} = \text{maximum}, \quad \text{if } \bar{\theta}^{kn} \text{ lies on the boundary} \\ \text{or} \quad & \\ & \frac{\partial H^{kn}}{\partial \theta^{kn}} = 0, \quad \text{if } \bar{\theta}^{kn} \text{ is on interior point.} \end{aligned} \qquad (19)$$

Let $\bar{\theta}^{(k)}(t)$ and $\bar{\theta}^{kn}$ be the optimal decision vector functions of the kth continuous and discrete branch respectively and $\bar{x}^{(k)}(t)$ and $\bar{x}^{kn}$ be the corresponding optimal state vector functions of the kth branch. Then we have

$$\theta^{(k)}(t,\epsilon) = \bar{\theta}^{(k)}(t) + \epsilon\varphi^{(k)}(t) + 0(\epsilon^2). \qquad (20)$$

$$\theta^{kn} = \bar{\theta}^{kn} + \epsilon\varphi^{kn} + 0(\epsilon^2). \qquad (21)$$

and

$$x^{(k)}(t,\epsilon) = \bar{x}^{(k)}(t) + \epsilon y^{(k)}(t) + 0(\epsilon^2). \qquad (22)$$

$$x^{kn} = \bar{x}^{kn} + \epsilon y^{kn} + 0(\epsilon^2). \qquad (23)$$

By means of a Taylor series expansion, the variational equations are obtained as

$$\begin{aligned} \epsilon \frac{dy_i^{(k)}}{dt} = \sum_{j=1}^{s^{(k)}} \epsilon y_j^{(k)} \frac{\partial f_i^{(k)}(\bar{x}^{(k)};\bar{\theta}^{(k)})}{\partial x_j^{(k)}} + f_i^{(k)}(\bar{x}^{(k)};\theta^{(k)}) \\ - f_i^{(k)}(\bar{x}^{(k)};\bar{\theta}^{(k)}) + 0(\epsilon^2). \end{aligned} \qquad (24)$$

for each continuous branch, and as

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* It will be proved in Section IV that these two conditions are equivalent for the continuous branches.

$$\epsilon y_i^{kn} = \sum_{j=1}^{s} \epsilon y_j^{k(n-1)} \frac{\partial T_i^{kn}(\bar{x}^{k(n-1)};\bar{\theta}^{kn})}{\partial \bar{x}_j^{k(n-1)}} + T_i^{kn}(\bar{x}^{k(n-1)};\bar{\theta}^{kn})$$

$$T_i^{kn}(\bar{x}^{k(n-1)};\bar{\theta}^{kn}) + O(\epsilon^2) \qquad (25)$$

for each discrete branch.

The relationships between the variations of the state vectors of different branches at the junction points are obtained by expanding the junction equations in power of ϵy_i as follows:

(a) Separating points

i) If the first branch (entering stream) is continuous

$$\epsilon y_i^{(k)}(0) \quad \text{or} \quad \epsilon y_i^{k0} = \sum_{j=1}^{s^{(1)}} \epsilon y_j^{(1)}(T_1) \frac{\partial g_i^{(k)}}{\partial x_j^{(1)}} + O(\epsilon^2), \qquad (26)^*$$

$$i = 1, 2, \ldots, s^{(k)}$$

$$k = 2, 3, \ldots, N.$$

ii) If the first branch (entering stream) is discrete

$$\epsilon y_i^{(k)}(0) \quad \text{or} \quad \epsilon y_i^{k0} = \sum_{j=1}^{s^{(1)}} \epsilon y_j^{1N} \frac{\partial g_i^{(k)}}{\partial x_j^{1N}} + O(\epsilon^2), \qquad (27)$$

$$i = 1, 2, \ldots, s^{(k)}$$

$$k = 2, 3, \ldots, N.$$

(b) Combining points

$$\epsilon y_i^{(N)}(0) \quad \text{or} \quad \epsilon y_i^{N0} = \sum_{c'} \sum_{j=1}^{s^{(c')}} \epsilon y_j^{(c')}(T_{c'}) \frac{\partial g_i^{(N)}}{\partial x_j^{(c')}} +$$

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* For the kth continuous branch, the first term of the left hand side is considered, and for the kth discrete term, the second term.

$$+\sum_{d'}\sum_{j=1}^{s^{(d')}} \epsilon y_j^{d'N} \frac{\partial g_i^{(N)}}{\partial x_j^{d'N}} + 0(\epsilon^2), \qquad i = 1, 2, \ldots, s^{(N)}. \quad (28)$$

(c) Crossing points

$$\epsilon y_i^{(k)}(0) \text{ or } \epsilon y_i^{k0} = \sum_{c'}\sum_{j=1}^{s^{(c')}} \epsilon y_j^{(c')}(T_{c'}) \frac{\partial g_i^{(k)}}{\partial x_j^{(c')}}$$

$$+\sum_{d'}\sum_{j=1}^{s^{(d')}} \epsilon y_j^{d'N} \frac{\partial g_i^{(k)}}{\partial x_j^{d'N}} + 0(\epsilon^2), \quad (29)$$

$$i = 1, 2, \ldots, s^{(k)}$$

$$k = m+1, \ldots, N.$$

Since all the initial states of the process are given and fixed, one has

$$y_i^{(k)}(0) = y_i^{k0} = 0, \qquad \begin{array}{l} i = 1, 2, \ldots, s^{(k)} \\ k = 1, 2, \ldots, b\ . \end{array} \quad (30)$$

where b denotes the number of entering branches with fixed initial states.

For the continuous branches, consider the relation

$$\frac{d}{dt}\sum_{i=1}^{s^{(k)}} \epsilon y_i^{(k)} z_i^{(k)} = \sum_{i=1}^{s^{(k)}} \epsilon z_i^{(k)} \frac{dy_i^{(k)}}{dt} + \sum_{i=1}^{s^{(k)}} \epsilon y_i^{(k)} \frac{dz_i^{(k)}}{dt}\ . \quad (31)$$

Substituting Equations (8) and (24) into (31) yields

$$\frac{d}{dt}\sum_{i=1}^{s^{(k)}} \epsilon y_i^{(k)} z_i^{(k)} = \sum_{i=1}^{s^{(k)}} z_i^{(k)} \left[f_i^{(k)}(\bar{x}^{(k)};\theta^{(k)}) - f_i^{(k)}(\bar{x}^{(k)};\bar{\theta}^{(k)}) \right] + 0(\epsilon^2). \quad (32)$$

Integrating Equation (32) from $t = 0$ to $t = T_k$, one obtains

$$\epsilon \sum_{i=1}^{s^{(k)}} \left[y_i^{(k)}(T_k)\, z_i^{(k)}(T_k) - y_i^{(k)}(0)\, z_i^{(k)}(0) \right]$$

$$= \int_0^T \sum_{i=1}^{s^{(k)}} z_i^{(k)} \left[f_i^{(k)}(\bar{x}^{(k)};\theta^{(k)}) - f_i^{(k)}(\bar{x}^{(k)};\bar{\theta}^{(k)}) \right] dt + 0(\epsilon^2). \quad (33)$$

For the discrete branches, multiplying Equation (25) by z_i^{kn} employing Equation (10), and summing from $n = 1$ to $n = N$ and $i = 1$ to $i = s^{(k)}$ give

$$\epsilon \sum_{i=1}^{s^{(k)}} (y_i^{kN} z_i^{kN} - y_i^{k0} z_i^{k0})$$

$$= \sum_{n=1}^{N} \sum_{i=1}^{s^{(k)}} z_i^{kn} \left[T_i^{kn}(\bar{x}^{k(n-1)}; \theta^{kn}) - T_i^{kn}(\bar{x}^{k(n-1)}; \bar{\theta}^{kn}) \right] + O(\epsilon^2) \ . \qquad (34)^*$$

Summing Equations (33) and (34) over all the continuous and discrete branches respectively and adding the resulting equations, one has

$$\sum_c \sum_{i=1}^{s^{(c)}} \epsilon \left[y_i^{(c)}(T_c)\, z_i^{(c)}(T_c) - y_i^{(c)}(0)\, z_i^{(c)}(0) \right] + \sum_d \sum_{i=1}^{s^{(d)}} \epsilon \left[y_i^{dN} z_i^{dN} - y_i^{d0} z_i^{d0} \right]$$

$$= \sum_c \int_0^T \sum_{i=1}^{s^{(c)}} z_i^{(c)} \left[f_i^{(c)}(\bar{x}^{(c)}; \theta^{(c)}) - f_i^{(c)}(\bar{x}^{(c)}; \bar{\theta}^{(c)}) \right] dt$$

$$+ \sum_d \sum_{n=1}^{N} \sum_{i=1}^{s^{(d)}} z_i^{dn} \left[T_i^{dn}(\bar{x}^{d(n-1)}; \theta^{dn}) - T_i^{dn}(\bar{x}^{d(n-1)}; \bar{\theta}^{dn}) \right] + O(\epsilon^2). \qquad (35)$$

For the branches containing the initial points or states, one has in the left hand side of Equation (35)

$$\epsilon y_i^{(k)}(0)\, z_i^{(k)}(0) = 0 \ ,$$

and $\qquad k = 1, 2, \ldots, b \qquad (36)$

$$\epsilon y_i^{k0} z_i^{k0} = 0 \ .$$

In the following, the three basic types are considered separately. It will be shown that they lead to the same conclusion, namely Equations (18) and (19). For those branches connected to a separating point, if the entering stream is continuous, one has from Equations (11) and (26)

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* $\bar{x}^{k(n-1)}$ indicates the optimal value of $x^{k(n-1)}$.

$$\sum_{c''} \sum_{i=1}^{s^{(c'')}} \epsilon y_i^{(c'')}(0)\, z_i^{(c'')}(0) + \sum_{d''} \sum_{i=1}^{s^{(d'')}} \epsilon y_i^{d''0}\, z_i^{d''0}$$

$$= \sum_{c''} \sum_{i=1}^{s^{(c'')}} \sum_{j=1}^{s^{(1)}} \epsilon y_j^{(1)}(T_1) \frac{\partial g_i^{(c'')}}{\partial x_j^{(1)}} z_i^{(c'')}(0)$$

$$+ \sum_{d''} \sum_{i=1}^{s^{(d'')}} \sum_{j=1}^{s^{(1)}} \epsilon y_j^{(1)}(T_1) \frac{\partial g_i^{(d'')}}{\partial x_j^{(1)}} z_i^{d''0}$$

$$= \sum_{j=1}^{s^{(1)}} \epsilon y_j^{(1)}(T_1) \left\lfloor \sum_{c''} \sum_{i=1}^{s^{(c'')}} \frac{\partial g_i^{(c'')}}{\partial x_j^{(1)}} z_i^{(c'')}(0) + \sum_{d''} \sum_{i=1}^{s^{(d'')}} \frac{\partial g_i^{(d'')}}{\partial x_j^{(1)}} z_i^{d''0} \right\rfloor$$

$$= \sum_{j=1}^{s^{(1)}} \epsilon y_j^{(1)}(T_1)\, z_j^{(1)}(T_1) = \sum_{i=1}^{s^{(1)}} \epsilon y_i^{(1)}(T_1)\, z_i^{(1)}(T_1) \, . \tag{37}$$

The left hand side of Equation (35) becomes, by using Equations (36) and (37).

$$\sum_{c''} \sum_{i=1}^{s^{(c'')}} \epsilon \left\lfloor y_i^{(c'')}(T_{c''})\, z_i^{(c'')}(T_{c''}) - y_i^{(c'')}(0)\, z_i^{(c'')}(0) \right\rfloor + \sum_{d''} \sum_{i=1}^{s^{(d'')}} \epsilon \left\lfloor y_i^{d''N}\, z_i^{d''N} \right.$$

$$\left. - y_i^{d''0}\, z_i^{d''0} \right\rfloor + \sum_{i=1}^{s^{(1)}} \epsilon \left\lfloor y_i^{(1)}(T_1)\, z_i^{(1)}(T_1) - y_i^{(1)}(0)\, z_i^{(1)}(0) \right\rfloor$$

$$= \sum_{c''} \sum_{i=1}^{s^{(c'')}} \epsilon y_i^{(c'')}(T_{c''})\, z_i^{(c'')}(T_{c''}) + \sum_{d''} \sum_{i=1}^{s^{(d'')}} \epsilon y_i^{d''N}\, z_i^{d''N} \, . \tag{38}$$

where the last bracketed quantity on the left hand side of Equation (38) is separated from the first bracketed quantity on the left hand side of Equation (35). Recall that $d'' = d$ for this case. Equation (35) thus becomes

$$\sum_{c''} \sum_{i=1}^{s^{(c'')}} \epsilon y_i^{(c'')}(T_{c''})\, z_i^{(c'')}(T_{c''}) + \sum_{d''} \sum_{i=1}^{s^{(d'')}} \epsilon y_i^{d''N}\, z_i^{d''N}$$

$$= \sum_c \int_0^T \sum_{i=1}^{s^{(c)}} z_i^{(c)} \left\lfloor f_i^{(c)}(\bar{x}^{(c)};\theta^{(c)}) - f_i^{(c)}(\bar{x}^{(c)};\bar{\theta}^{(c)}) \right\rfloor dt$$

$$+ \sum_d \sum_{n=1}^{N} \sum_{i=1}^{s^{(d)}} z_i^{dn} \left\lfloor T_i^{dn}(\bar{x}^{d(n-1)};\theta^{dn}) - T_i^{dn}(\bar{x}^{d(n-1)};\bar{\theta}^{dn}) \right\rfloor + 0(\epsilon^2). \qquad (39)$$

If the objective function is to be maximized, the perturbation of the decision variables can only be to make

$$\left\lfloor \sum_{c''} \sum_{i=1}^{s^{(c'')}} \epsilon c_i^{(c'')} y_i^{(c'')}(T_{c''}) + \sum_{d''} \sum_{i=1}^{s^{(d'')}} \epsilon c_i^{d''N} \, y_i^{d''N} \right\rfloor \leq 0 \ . \qquad (40)$$

Combining Equations (17), (39), and (40) gives

$$\sum_c \int_0^T \sum_{i=1}^{s^{(c)}} z_i^{(c)} \left\lfloor f_i^{(c)}(\bar{x}^{(c)};\theta^{(c)}) - f_i^{(c)}(\bar{x}^{(c)};\bar{\theta}^{(c)}) \right\rfloor dt$$

$$+ \sum_d \sum_{n=1}^{N} \sum_{i=1}^{s^{(d)}} z_i^{dn} \left\lfloor T_i^{dn}(\bar{x}^{d(n-1)};\theta^{dn}) - T_i^{dn}(\bar{x}^{d(n-1)};\bar{\theta}^{dn}) \right\rfloor + 0(\epsilon^2) \leq 0. \quad (41)$$

or

$$\sum_c \int_0^T \sum_{i=1}^{s^{(c)}} z_i^{(c)} \left\lfloor f_i^{(c)}(\bar{x}^{(c)};\theta^{(c)}) - f_i^{(c)}(\bar{x}^{(c)};\theta^{(c)}) \right\rfloor dt$$

$$+ \sum_d \sum_{n=1}^{N} \sum_{i=1}^{s^{(1)}} z_i^{dn} \left\lfloor \sum_{j=1}^{r} \epsilon \varphi_j^{dn} \frac{\partial T_i^{dn}(\bar{x}^{d(n-1)};\bar{\theta}^{dn})}{\partial \bar{\theta}_j^{dn}} \right\rfloor + 0(\epsilon^2) \leq 0 \ . \qquad (42)$$

Since the perturbation of each decision vector is independent of the perturbations in the other decision vectors both in the continuous branches and in the stages of each discrete branch, it may be concluded that the integrand of each integral and each term containing a set of independent variables must itself be non-positive. Thus

$$\sum_{i=1}^{s^{(c)}} z_i^{(c)} \left\lfloor f_i^{(c)}(\bar{x}^{(c)};\theta^{(c)}) - f_i^{(c)}(\bar{x}^{(c)};\bar{\theta}^{(c)}) \right\rfloor + 0(\epsilon^2) \leq 0 \ , \qquad (43)$$

and

$$\sum_{j=1}^{r} (\theta_j^{dn} - \bar{\theta}_j^{dn}) \sum_{i=1}^{s^{(d)}} z_i^{dn} \frac{\partial T_i^{dn}(\bar{x}^{d(n-1)};\bar{\theta}^{dn})}{\partial \bar{\theta}_j^{dn}} + O(\epsilon^2) \leq 0 , \qquad (44)$$

which are equivalent to Equations (18) and (19).

For those branches connected to a separating point, if the entering stream is discrete, one has by using Equations (12) and (27)

$$\sum_{c''} \sum_{i=1}^{s^{(c'')}} \epsilon y_i^{(c'')}(0)\, z_i^{(c'')}(0) + \sum_{d''} \sum_{i=1}^{s^{(d'')}} \epsilon y_i^{d''0}\, z_i^{d''0}$$

$$= \sum_{c''} \sum_{i=1}^{s^{(c'')}} \sum_{j=1}^{s^{(1)}} \epsilon y_j^{1N} \frac{\partial g_i^{(c'')}}{\partial x_j^{1N}} z_i^{(c'')}(0) + \sum_{d''} \sum_{i=1}^{s^{(d'')}} \sum_{j=1}^{s^{(1)}} \epsilon y_j^{1N} \frac{\partial g_i^{(d'')}}{\partial x_j^{1N}} z_i^{d''0}$$

$$= \sum_{j=1}^{s^{(1)}} \epsilon y_j^{1N} \left[\sum_{c''} \sum_{j=1}^{s^{(c'')}} \frac{\partial g_i^{(c'')}}{\partial x_j^{1N}} z_i^{(c'')}(0) + \sum_{d''} \sum_{i=1}^{s^{(d'')}} \frac{\partial g_i^{(d'')}}{\partial x_j^{1N}} z_i^{d''0} \right]$$

$$= \sum_{j=1}^{s^{(1)}} \epsilon y_j^{1N} z_j^{1N} = \sum_{i=1}^{s^{(1)}} \epsilon y_i^{1N} z_i^{1N} . \qquad (45)$$

By using Equations (36) and (45), Equation (35) is reduced to

$$\sum_{d''} \sum_{i=1}^{s^{(d'')}} \epsilon y_i^{d''N} z_i^{d''N} + \sum_{c''} \sum_{i=1}^{s^{(c'')}} \epsilon y_i^{(c'')}(T_{c''})\, z_i^{(c'')}(T_{c''})$$

$$= \sum_{d} \sum_{n=1}^{N} \sum_{i=1}^{s^{(d)}} z_i^{dn} \left[T_i^{dn}(\bar{x}^{d(n-1)};\theta^{dn}) - T_i^{dn}(\bar{x}^{d(n-1)};\bar{\theta}^{dn}) \right]$$

$$+ \sum_{c} \int_0^T \sum_{i=1}^{s^{(c)}} z_i^{(c)} \left[f_i^{(c)}(\bar{x}^{(c)};\theta^{(c)}) - f_i^{(c)}(\bar{x}^{(c)};\bar{\theta}^{(c)}) \right] dt + O(\epsilon^2). \qquad (46)$$

It is worth recalling that $c'' = c$ for this case.

If the objective function is to be maximized, the perturbation of the decision variables can only be to make

$$\left[\sum_{d''} \sum_{i=1}^{s^{(d'')}} \epsilon c_i^{d''N} y_i^{d''N} + \sum_{c''} \sum_{i=1}^{s^{(c'')}} \epsilon c_i^{(c'')} y_i^{(c'')}(T_{c''})\right] + 0(\epsilon^2) \leq 0, \quad (47)$$

or

$$\sum_{d} \sum_{n=1}^{N} \sum_{i=1}^{s^{(d)}} z_i^{dn} \left[T_i^{dn}(\bar{x}^{d(n-1)};\theta^{dn}) - T_i^{dn}(\bar{x}^{d(n-1)};\bar{\theta}^{dn})\right] + 0(\epsilon^2) \leq 0 , \quad (48)$$

and

$$\sum_{c} \int_0^T \sum_{i=1}^{s^{(c)}} z_i^{(c)} \left[f_i^{(c)}(\bar{x}^{(c)};\theta^{(c)}) - f_i^{(c)}(\bar{x}^{(c)};\bar{\theta}^{(c)})\right] dt + 0(\epsilon^2) \leq 0. \quad (49)$$

Following a similar reasoning as before, one has

$$\sum_{i=1}^{s^{(c)}} z_i^{(c)} \left[f_i^{(c)}(\bar{x}^{(c)};\theta^{(c)}) - f_i^{(c)}(\bar{x}^{(c)};\bar{\theta}^{(c)})\right] + 0(\epsilon^2) \leq 0 , \quad (50)$$

and

$$\sum_{j=1}^{r} (\theta_j^{dn} - \bar{\theta}_j^{dn}) \sum_{i=1}^{s^{(d)}} z_i^{dn} \frac{\partial T_i^{dn}(\bar{x}^{d(n-1)};\bar{\theta}^{dn})}{\partial \bar{\theta}_j^{dn}} + 0(\epsilon^2) \leq 0 . \quad (51)$$

For those branches connected to a combining point, if the leaving branch is continuous, one has from Equations (13), (14), and (28)

$$\sum_{i=1}^{s^{(N)}} \epsilon y_i^{(N)}(0) z_i^{(N)}(0) = \sum_{i=1}^{s^{(N)}} \left[\sum_{c'} \sum_{j=1}^{s^{(c')}} \epsilon y_j^{(c')}(T_{c'}) \frac{\partial g_i^{(N)}}{\partial x_j^{(c')}} + \sum_{d'} \sum_{j=1}^{s^{(d')}} \epsilon y_j^{d'N} \frac{\partial g_i^{(N)}}{\partial x_j^{d'N}}\right] z_i^{(N)}(0)$$

$$= \sum_{c'} \sum_{i=1}^{s^{(N)}} \sum_{j=1}^{s^{(c')}} \epsilon y_j^{(c')}(T_{c'}) \frac{\partial g_i^{(N)}}{\partial x_j^{(c')}} z_i^{(N)}(0) + \sum_{d'} \sum_{i=1}^{s^{(N)}} \sum_{j=1}^{s^{(d')}} \epsilon y_j^{d'N} \frac{\partial g_i^{(N)}}{\partial x_j^{d'N}} z_i^{(N)}(0)$$

$$= \sum_{c'} \sum_{j=1}^{s^{(c')}} \epsilon y_j^{(c')}(T_{c'}) \sum_{i=1}^{s^{(N)}} \frac{\partial g_i^{(N)}}{\partial x_j^{(c')}} z_i^{(N)}(0) + \sum_{d'} \sum_{j=1}^{s^{(d')}} \epsilon y_j^{d'N} \sum_{i=1}^{s^{(N)}} \frac{\partial g_i^{(N)}}{\partial x_j^{d'N}} z_i^{(N)}(0)$$

$$= \sum_{c'} \sum_{j=1}^{s^{(c')}} \epsilon y_j^{(c')}(T_{c'})\, z_i^{(c')}(T_{c'}) + \sum_{d'} \sum_{j=1}^{s^{(d')}} \epsilon y_j^{d'N}\, z_j^{d'N} \,. \tag{52}$$

Recall that, for this case, $d' = d$. The left hand side of Equation (35) becomes by using Equations (36) and (52)

$$\sum_c \sum_{i=1}^{s^{(c)}} \epsilon\left[y_i^{(c)}(T_c)\, z_i^{(c)}(T_c) - y_i^{(c)}(0)\, z_i^{(c)}(0)\right]$$

$$+ \sum_d \sum_{i=1}^{s^{(d)}} \epsilon\left[y_i^{dN}\, z_i^{dN} - y_i^{d0}\, z_i^{d0}\right]$$

$$= \sum_{i=1}^{s^{(N)}} \epsilon y_i^{(N)}(T_N)\, z_i^{(N)}(T_N) + \sum_{c'} \sum_{i=1}^{s^{(c')}} \epsilon y_i^{(c')}(T_{c'})\, z_i^{(c')}(T_{c'})$$

$$- \sum_{i=1}^{s^{(N)}} \epsilon y_i^{(N)}(0)\, z_i^{(N)}(0) - \sum_{c'} \sum_{i=1}^{s^{(c')}} \epsilon y_i^{(c')}(0)\, z_i^{(c')}(0)$$

$$+ \sum_{d'} \sum_{i=1}^{s^{(d')}} \epsilon\left[y_i^{d'N}\, z_i^{d'N} - y_i^{d'0}\, z_i^{d'0}\right]$$

$$= \sum_{i=1}^{s^{(N)}} \epsilon y_i^{(N)}(T_N)\, z_i^{(N)}(T_N) \,. \tag{53}$$

Equating this to the right hand side of Equation (35) gives

$$\sum_{i=1}^{s^{(N)}} \epsilon y_i^{(N)}(T_N)\, z_i^{(N)}(T_N)$$

$$= \sum_c \int_0^T \sum_{i=1}^{s^{(c)}} z_i^{(c)}\left[f_i^{(c)}(\bar{x}^{(c)};\theta^{(c)}) - f_i^{(c)}(\bar{x}^{(c)};\bar{\theta}^{(c)})\right] dt$$

$$+ \sum_d \sum_{n=1}^{N} \sum_{i=1}^{s^{(d)}} z_i^{dn}\left[T_i^{dn}(\bar{x}^{d(n-1)};\theta^{dn}) - T_i^{dn}(\bar{x}^{d(n-1)};\bar{\theta}^{dn})\right] + O(\epsilon^2). \tag{54}$$

If the objective function is to be maximized, the perturbation of the

decision variables can only be to make

$$\sum_{i=1}^{s^{(N)}} \epsilon c_i^{(N)} \, y_i^{(N)} \leq 0 \quad , \tag{55}$$

or

$$\sum_{i=1}^{s^{(c)}} z_i^{(c)} \Big[f_i^{(c)}(\bar{x}^{(c)};\theta^{(c)}) - f_i^{(c)}(\bar{x}^{(c)};\bar{\theta}^{(c)}) \Big] + O(\epsilon^2) \leq 0 \tag{56}$$

$$\sum_{j=1}^{r} (\theta_j^{dn} - \bar{\theta}_j^{dn}) \sum_{i=1}^{s^{(d)}} z_i^{dn} \frac{\partial T_i^{dn}(\bar{x}^{d(n-1)};\bar{\theta}^{dn})}{\partial \bar{\theta}_j^{dn}} + O(\epsilon^2) \leq 0 \ . \tag{57}$$

If the leaving stream is discrete, by using Equations (13), (14), and (28) one has

$$\begin{aligned}
&\sum_{i=1}^{s^{(N)}} \epsilon y_i^{NO} \, z_i^{NO} \\
&= \sum_{i=1}^{s^{(N)}} \Big[\sum_{c'} \sum_{j=1}^{s^{(c')}} \epsilon y_j^{(c')}(T_{c'}) \frac{\partial g_i^{(N)}}{\partial x_j^{(c')}} + \sum_{d'} \sum_{j=1}^{s^{(d')}} \epsilon y_j^{d'N} \frac{\partial g_i^{(N)}}{\partial x_j^{d'N}} \Big] z_i^{NO} \\
&= \sum_{c'} \sum_{i=1}^{s^{(N)}} \sum_{j=1}^{s^{(c')}} \epsilon y_j^{(c')}(T_{c'}) \frac{\partial g_i^{(N)}}{\partial x_j^{(c')}} z_i^{NO} + \sum_{d'} \sum_{i=1}^{s^{(N)}} \sum_{j=1}^{s^{(d')}} \epsilon y_j^{d'N} \frac{\partial g_i^{(N)}}{\partial x_j^{d'N}} z_i^{NO} \\
&= \sum_{c'} \sum_{j=1}^{s^{(c')}} \epsilon y_j^{(c')}(T_{c'}) \sum_{i=1}^{s^{(N)}} \frac{\partial g_i^{(N)}}{\partial x_j^{(c')}} z_i^{NO} + \sum_{d'} \sum_{j=1}^{s^{(d')}} \epsilon y_j^{d'N} \sum_{i=1}^{s^{(N)}} \frac{\partial g_i^{(N)}}{\partial x_j^{d'N}} z_i^{NO} \\
&= \sum_{c'} \sum_{j=1}^{s^{(c')}} \epsilon y_j^{(c')}(T_{c'}) \, z_j^{(c')}(T_{c'}) + \sum_{d'} \sum_{j=1}^{s^{(d')}} \epsilon y_j^{d'N} \, z_j^{d'N} \ .
\end{aligned} \tag{58}$$

Note that, for this case, $c' = c$. By using Equations (36) and (58), the left hand side of Equation (35) becomes

$$\sum_{c} \sum_{i=1}^{s^{(c)}} \epsilon \Big[y_i^{(c)}(T_c) z_i^{(c)}(T_c) - y_i^{(c)}(0) z_i^{(c)}(0) \Big] + \sum_{d} \sum_{i=1}^{s^{(d)}} \epsilon \Big[y_i^{dN} z_i^{dN} - y_i^{d0} z_i^{d0} \Big]$$

$$= \sum_{c'} \sum_{i=1}^{s^{(c')}} \epsilon y_i^{(c')}(T_{c'})\, z_i^{(c')}(T_{c'}) + \sum_{i=1}^{s^{(N)}} \epsilon y_i^{NN}\, z_i^{NN}$$

$$+ \sum_{d'} \sum_{i=1}^{s^{(d')}} \epsilon y_i^{d'N}\, z_i^{d'N} - \sum_{i=1}^{s^{(N)}} \epsilon y_i^{NO}\, z_i^{NO}$$

$$= \sum_{c'} \sum_{i=1}^{s^{(c')}} \epsilon y_i^{(c')}(T_{c'}) z_i^{(c')}(T_{c'}) + \sum_{i=1}^{s^{(N)}} \epsilon y_i^{NN} z_i^{NN} + \sum_{d'} \sum_{i=1}^{s^{(d')}} \epsilon y_i^{d'N} z_i^{d'N}$$

$$= \sum_{c'} \sum_{j=1}^{s^{(c')}} \epsilon y_j^{(c')}(T_{c'})\, z_j^{(c')}(T_{c'}) - \sum_{d'} \sum_{j=1}^{s^{(d')}} \epsilon y_j^{d'N}\, z_j^{d'N}$$

$$= \sum_{i=1}^{s^{(N)}} \epsilon y_i^{NN}\, z_i^{NN} . \tag{59}$$

Equating this to the right hand side of Equation (35) gives

$$\sum_{i=1}^{s^{(N)}} \epsilon y_i^{NN}\, z_i^{NN} = \sum_c \int_0^T \sum_{i=1}^{s^{(c)}} z^{(c)} \left[f_i^{(c)}(\bar{x}^{(c)};\theta^{(c)}) - f_i^{(c)}(\bar{x}^{(c)};\bar{\theta}^{(c)}) \right] dt$$

$$+ \sum_d \sum_{n=1}^{N} \sum_{i=1}^{s^{(d)}} z_i^{dn} \left[T_i^{dn}(\bar{x}^{d(n-1)};\theta^{dn}) - T_i^{dn}(\bar{x}^{d(n-1)};\bar{\theta}^{d(n)}) \right] + 0(\epsilon^2). \tag{60}$$

Therefore

$$\sum_{i=1}^{s^{(c)}} z_i^{(c)} \left[f_i^{(c)}(\bar{x}^{(c)};\theta^{(c)}) - f_i^{(c)}(\bar{x}^{(c)};\bar{\theta}^{(c)}) \right] + 0(\epsilon^2) \leq 0 \quad , \tag{61}$$

and

$$\sum_{j=1}^{r^{(d)}} (\theta_j^{dn} - \bar{\theta}_j^{dn}) \sum_{i=1}^{s^{(d)}} z_i^{dn} \frac{\partial T_i^{dn}(\bar{x}^{d(n-1)};\bar{\theta}^{dn})}{\partial \bar{\theta}_j^{dn}} + 0(\epsilon^2) \leq 0 . \tag{62}$$

which are equivalent to Equations (18) and (19).

For those branches connected to a crossing point, by using Equations (15), (16) and (29), and recalling that $\sum_{c'}$ sums over all the entering

streams that are continuous, $\Sigma_{d'}$ sums over all the entering streams which are discrete and $\Sigma_{c''}$ and $\Sigma_{d''}$ sum over all the continuous and discrete leaving streams respectively, one has

$$\sum_{c''}\sum_{i=1}^{s^{(c'')}} \epsilon y_i^{(c'')}(0)\, z_i^{(c'')}(0) + \sum_{d''}\sum_{i=1}^{s^{(d'')}} \epsilon y_i^{d''0}\, z_i^{d''0}$$

$$= \sum_{c''}\sum_{i=1}^{s^{(c'')}} \left[\sum_{c'}\sum_{j=1}^{s^{(c')}} \epsilon y_j^{(c')}(T_{c'}) \frac{\partial g_i^{(c')}}{\partial x_j^{(c')}} + \sum_{d'}\sum_{j=1}^{s^{(d')}} \epsilon y_j^{d'N} \frac{\partial g_i^{(d')}}{\partial x_j^{d'N}}\right] z_i^{(c'')}(0)$$

$$+ \sum_{d''}\sum_{i=1}^{s^{(d'')}} \left[\sum_{c'}\sum_{j=1}^{s^{(c')}} \epsilon y_j^{(c')}(T_{c'}) \frac{\partial g_i^{(d'')}}{\partial x_j^{(c')}} + \sum_{d'}\sum_{j=1}^{s^{(d')}} \epsilon y_j^{d'N} \frac{\partial g_i^{(d'')}}{\partial x_j^{d'N}}\right] z_i^{d''0}$$

$$= \sum_{c'}\sum_{j=1}^{s^{(c')}} \epsilon y_j^{(c')}(T_{c'})\, z_j^{(c')}(T_{c'}) + \sum_{d'}\sum_{j=1}^{s^{(d')}} \epsilon y_j^{d'N}\, z_j^{d'N}$$

$$= \sum_{c'}\sum_{j=1}^{s^{(c')}} \epsilon y_j^{(c')}(T_{c'})\, z_j^{(c')}(T_{c'}) + \sum_{d'}\sum_{j=1}^{s^{(d')}} \epsilon y_j^{d'N}\, z_j^{d'N} \,. \tag{63}$$

By using Equations (36) and (63) the left hand side of Equation (35) can be written as

$$\sum_{c}\sum_{i=1}^{s^{(c)}} \epsilon\left[y_i^{(c)}(T_c)\, z_i^{(c)}(T_c) - y_i^{(c)}(0)\, z_i^{(c)}(0)\right]$$

$$+ \sum_{d}\sum_{i=1}^{s^{(d)}} \epsilon\left[y_i^{dN}\, z_i^{dN} - y_i^{d0}\, z_i^{d0}\right]$$

$$= \sum_{c'}\sum_{i=1}^{s^{(c')}} \epsilon y_i^{(c')}(T_{c'})\, z_i^{(c')}(T_{c'}) + \sum_{c''}\sum_{i=1}^{s^{(c'')}} \epsilon y_i^{(c'')}(T_{c''})\, z_i^{(c'')}(T_{c''})$$

$$+ \sum_{d'}\sum_{i=1}^{s^{(d')}} \epsilon y_i^{d''N}\, z_i^{d''N} + \sum_{d''}\sum_{i=1}^{s^{(d'')}} \epsilon y_i^{d''N}\, z_i^{d''N}$$

$$= \left[\sum_{c''} \sum_{i=1}^{s^{(c'')}} \epsilon y_i^{(c'')}(0)\, z_i^{(c'')}(0) + \sum_{d''} \sum_{i=1}^{s^{(d'')}} \epsilon y_i^{d''0}\, z_i^{d''0}\right]$$

$$= \sum_{c''} \sum_{i=1}^{s^{(c'')}} \epsilon y_i^{(c'')}(T_{c''})\, z_i^{(c'')}(T_{c''}) + \sum_{d''} \sum_{i=1}^{s^{(d'')}} \epsilon y_i^{d''N}\, z_i^{d''N} \quad . \tag{64}$$

It is worth recalling that

$$c = c' + c''$$

$$d = d' + d''$$

$$N = c + d$$

Equating the right hand side of Equation (64) and the right hand side of Equation (35) gives

$$\sum_{c''} \sum_{i=1}^{s^{(c'')}} \epsilon y_i^{(c'')}(T_{c''})\, z_i^{(c'')}(T_{c''}) + \sum_{d''} \sum_{i=1}^{s^{(d'')}} \epsilon y_i^{d''N}\, z_i^{d''N}$$

$$= \sum_{c} \int_0^T \sum_{i=1}^{s^{(c)}} z_i^{(c)}\left[f_i^{(c)}(\bar{x}^{(c)};\theta^{(c)}) - f_i^{(c)}(\bar{x}^{(c)};\bar{\theta}^{(c)})\right] dt$$

$$+ \sum_{d} \sum_{n=1}^{N} \sum_{i=1}^{s^{(d)}} z_i^{dn}\left[T_i^{dn}(\bar{x}^{d(n-1)};\theta^{dn}) - T_i^{dn}(\bar{x}^{d(n-1)};\bar{\theta}^{dn})\right] + 0(\epsilon^2). \tag{65}$$

Similarly, if the objective function is to be maximized, the perturbation of the decision variables can only be to make

$$\sum_{i=1}^{s^{(d'')}} \epsilon c_i^{d''N}\, y_i^{d''N} \le 0 \quad . \tag{66}$$

and

$$\sum_{i=1}^{s^{(c'')}} \epsilon c_i^{(c'')} y_i^{(c'')}(T_{c''}) \le 0 \quad , \tag{67}$$

or

$$\sum_{i=1}^{s^{(c)}} z_i^{(c)} \left[f_i^{(c)}(\bar{x}^{(c)};\theta^{(c)}) - f_i^{(c)}(\bar{x}^{(c)};\bar{\theta}^{(c)}) \right] + 0(\epsilon^2) \leq 0 \ , \qquad (68)$$

and

$$\sum_{j=1}^{r} (\theta_j^{dn} - \bar{\theta}_j^{dn}) \sum_{i=1}^{s^{(d)}} z_i^{dn} \frac{\partial T_i^{dn}(\bar{x}^{d(n-1)};\bar{\theta}^{dn})}{\partial \bar{\theta}_j^{dn}} + 0(\epsilon^2) \leq 0 \ . \qquad (69)$$

Equations (68) and (69) are equivalent to Equations (18) and (19).

Applications

1. A simple composite process. For illustrating the use of the algorithm for composite processes, let us consider the problem which has been solved by using a sequential union of the maximum principle and dynamic programming (9). The composite process consists of a discrete unit and a continuous unit as shown in Figure 6. For the discrete unit

$$\begin{aligned} x_1^{11} &= x_1^{10} + \theta^{11} \ , \\ x_1^{10} &= \gamma \ . \end{aligned} \qquad (70)$$

For the continuous unit

$$\begin{aligned} \frac{dx_1^{(2)}}{dt} &= - ax_1^{(2)} + \theta^{(2)} \ , \\ x_1^{(2)}(0) &= x_1^{11} \ . \end{aligned} \qquad (71)$$

It is desired to minimize the total cost

$$p^{(1)} + p^{(2)}$$

where

$$p^{(1)} = x_1^{11} = \mu\theta^{11} \ , \qquad (72)$$

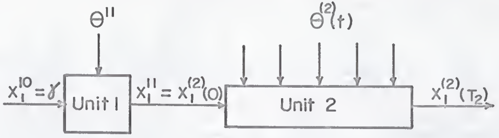


Fig. 6. A simple composite process.

$$p^{(2)} = \frac{1}{2}\int_0^{T_2} \left[(x_1^{(2)})^2 + (\theta_2^{(2)})^2\right] dt . \tag{73}$$

To solve this problem, an additional state variable is introduced such that

$$x_2^{11} = x_1^{11} - \mu\theta^{11}$$

and

$$x_2^{(2)}(t) = \frac{1}{2}\int_0^{t} \left[(x_1^{(2)})^2 + (\theta^{(2)})^2\right] dt + x_2^{11} . \tag{74}$$

This gives

$$\frac{dx_2^{(2)}}{dt} = \frac{1}{2}\left[(x_1^{(2)})^2 + (\theta^{(2)})^2\right] , \tag{75}$$

and

$$x_2^{(2)}(0) = x_2^{11} . \tag{76}$$

Hence, for the continuous branch, one has

$$H^{(2)} = z_1^{(2)}\left[- ax_1^{(2)} + \theta^{(2)}\right] + z_2^{(2)}\left[\frac{1}{2}(x_1^{(2)})^2 + \frac{1}{2}(\theta^{(2)})^2\right] , \tag{77}$$

$$\frac{dz_1^{(2)}}{dt} = - \frac{\partial H^{(2)}}{\partial x_1^{(2)}} = az_1^{(2)} - z_2^{(2)}\, x_1^{(2)}, \qquad z_1^{(2)}(T_2) = 0 , \tag{78}$$

$$\frac{dz_2^{(2)}}{dt} = - \frac{\partial H^{(2)}}{\partial x_2^{(2)}} = 0 , \qquad z_2^{(2)}(T) = 1 . \tag{79}$$

It follows from Equation (79) that

$$z_2^{(2)}(t) = 1 .$$

Assuming that the Hamiltonian attains its minimum at an interior point of the region of $\theta(t)$, we obtain the optimal decision by setting

$$\frac{\partial H^{(2)}}{\partial \theta^{(2)}} = 0 ,$$

which gives

$$\theta^{(2)}(t) = - z(t) = \bar{\theta}(t) \ . \tag{80}$$

The corresponding x(t) and z(t) are found from Equations (71) and (78) as

$$x_1^{(2)}(t) = x_1^{11} \left\lfloor \alpha e^{\lambda t} + \beta e^{-\lambda t} \right\rfloor , \tag{81}$$

$$z_1^{(2)}(t) = x_1^{11} \left\lfloor \alpha(\lambda+a)e^{\lambda t} - \beta(\lambda-a)e^{-\lambda t} \right\rfloor , \tag{82}$$

where

$$\lambda = \sqrt{a^2 + 1} \ ,$$

α, β are constants which can be determined from the boundary conditions

$$x_1^{11} = x_1^{(2)}(0) \ ,$$

and

$$z_1^{(2)}(T_2) = 0 \ .$$

The junction equations are

$$x_1^{(2)}(0) = x_1^{11} \ ,$$

$$x_2^{(2)}(0) = x_2^{11} \ .$$

Hence, by using Equation (14), one obtains

$$\begin{aligned} z_1^{11} &= z_1^{(2)}(0) \ , \\ z_2^{11} &= z_2^{(2)}(0) = 1 \ . \end{aligned} \tag{83}$$

The Hamiltonian for the discrete unit is

$$\begin{aligned} H^{11} &= z_1^{11} \left\lfloor x_1^{10} + \theta^{11} \right\rfloor + z_2^{11} \left\lfloor x_1^{11} - \mu\theta^{11} \right\rfloor \\ &= z_1^{(2)}(0) \left\lfloor x_1^{10} + \theta^{11} \right\rfloor + (x_1^{10} + \theta^{11} - \mu\theta^{11}) \ . \end{aligned} \tag{84}$$

Assuming that H^{11} is stationary in the interior of the admissible range of

θ^{11}, one obtains the optimal decision from the necessary condition

$$\frac{\partial H^{11}}{\partial \theta^{11}} = 0 ,$$

which gives

$$z_1^{(2)}(0) = -(1-\mu) . \tag{85}$$

From Equation (82) one has

$$\begin{aligned} z_1^{(2)}(0) &= x_1^{11} \left\lfloor \alpha(\lambda+a) - \beta(\lambda-a) \right\rfloor \\ &= \left\lfloor x_1^{10} + \theta^{11} \right\rfloor \left\lfloor \alpha(\lambda+a) - \beta(\lambda-a) \right\rfloor . \end{aligned} \tag{86}$$

Solving for θ^{11} from Equations (85) and (86) gives

$$\begin{aligned} \bar{\theta}^{11} &= \frac{-(1-\mu)}{\alpha(\lambda+a) - \beta(\lambda-a)} - x_1^{10} \\ &= \frac{-(1-\mu)}{\alpha(\lambda+a) - \beta(\lambda-a)} - \gamma . \end{aligned} \tag{87}$$

The minimum cost is obtained by substituting Equations (80), (81), and (87) into Equations (72) and (73) and adding the resulting values as

$$p^{(1)} + p^{(2)} = \mu\gamma - \frac{1}{C} \left(\frac{\mu-1}{2}\right)^2 ,$$

where

$$C = \frac{1}{2} \left\lfloor \frac{e^{\lambda T_2} - e^{-\lambda T_2}}{(\lambda+a)e^{\lambda T_2} + (\lambda-a)e^{\lambda T_2}} \right\rfloor = \text{constant.}$$

2. Reactor system with recycle to an internal point. A first order consecutive chemical reaction

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

is carried out in the reactor system as shown in Figure 7. The initial

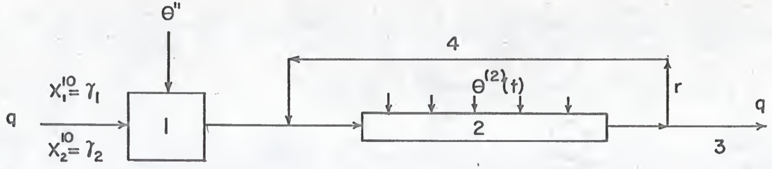


Fig. 7 A process with recycle to an internal point.

concentrations of the reactants, A and B are γ_1 and γ_2 respectively. It is desired to obtain the maximum yield of the intermediate product at the outlet of the system.

To illustrate the use of the working alforithms for composite processes, the optimal policy is obtained only in the form of differential equations.

For the first branch

$$x_1^{11} = x_1^{10} - t_1 k_{10} e^{-\frac{E_1}{R\theta^{11}}} x_1^{11} , \qquad x_1^{10} = \gamma_1 \tag{88}$$

$$x_2^{11} = x_2^{10} + t_1 \left[k_{10} e^{-\frac{E_1}{R\theta^{11}}} x_1^{11} - k_{20} e^{-\frac{E_2}{R\theta^{11}}} x_2^{11} \right], \qquad x_2^{10} = \gamma_2 \tag{89}$$

where t_1 is the residence time and is assumed to be constant. For the second branch

$$\frac{dx_1^{(2)}}{dt} = - k_{10} e^{-\frac{E_1}{R\theta^{(2)}}} x_1^{(2)} , \tag{90}$$

$$\frac{dx_2^{(2)}}{dt} = k_{10} e^{-\frac{E_1}{R\theta^{(2)}}} x_1^{(2)} - k_{20} e^{-\frac{E_2}{R\theta^{(2)}}} x_2^{(2)} . \tag{91}$$

For the third and fourth branch

$$\frac{dx_1^{(3)}}{dt} = 0 \quad , \quad \frac{dx_2^{(3)}}{dt} = 0 . \tag{92}$$

$$\frac{dx_1^{(4)}}{dt} = 0 \quad , \quad \frac{dx_2^{(4)}}{dt} = 0 . \tag{93}$$

The junction equations are

$$\begin{aligned} x_1^{(2)}(0) &= \alpha x_1^{11} + \beta x_1^{(4)}(T_4) , \\ x_2^{(2)}(0) &= \alpha x_2^{11} + \beta x_2^{(4)}(T_4) . \end{aligned} \tag{94}$$

where

$$\alpha = \frac{q}{q + r} \quad , \quad \beta = \frac{r}{q + r}$$

$$x_1^{(3)}(0) = x_1^{(3)}(T_3) = x_1^{(2)}(T_2) \ ,$$
$$x_2^{(3)}(0) = x_2^{(3)}(T_3) = x_2^{(2)}(T_2) \ , \tag{95}$$

$$x_1^{(4)}(0) = x_1^{(4)}(T_4) = x_1^{(2)}(T_2) \ ,$$
$$x_2^{(4)}(0) = x_2^{(4)}(T_4) = x_2^{(2)}(T_2) \ . \tag{96}$$

Then the objective function is

$$S = x_2^{(3)}(T_3) \ . \tag{97}$$

The Hamiltonian for each branch is

$$H^{11} = x_1^{11} \, z_1^{11} + z_2^{11} \, x_2^{11} \ , \tag{98}$$

$$H^{(2)} = z_1^{(2)} \frac{dx_1^{(2)}}{dt} + z_2^{(2)} \frac{dx_2^{(2)}}{dt}$$

$$= z_1^{(2)}(-k_{10} e^{-\frac{E_1}{R\theta^{(2)}}} x_1^{(2)}) + z_2^{(2)}(k_{10} e^{-\frac{E_1}{R\theta^{(2)}}} x_1^{(2)} - k_{20} e^{-\frac{E_2}{R\theta^{(2)}}} x_2^{(2)}) \ , \tag{99}$$

$$H^{(3)} = H^{(4)} = 0 \ . \tag{100}$$

The adjoint functions are

$$\frac{dz_1^{(2)}}{dt} = - \frac{\partial H^{(2)}}{\partial x_1^{(2)}} = z_1^{(2)} \, k_{10} e^{-\frac{E_1}{R\theta^{(2)}}} - z_2^{(2)} \, k_{10} e^{-\frac{E_1}{R\theta^{(2)}}}$$

$$= k_{10} e^{-\frac{E_1}{R\theta^{(2)}}} (z_1^{(2)} - z_2^{(2)}) , \tag{101}$$

$$\frac{dz_2^{(2)}}{dt} = - \frac{\partial H^{(2)}}{\partial x_2^{(2)}} = z_2^{(2)} \, k_{20} e^{-\frac{E_2}{R\theta^{(2)}}} , \tag{102}$$

$$\frac{dz_1^{(3)}}{dt} = \frac{dz_2^{(3)}}{dt} = \frac{dz_1^{(4)}}{dt} = \frac{dz_2^{(4)}}{dt} = 0 . \tag{103}$$

According to Equations (13), (14) and Equation (94), we have at the combining point

$$z_1^{11} = \alpha z_1^{(2)}(0) , \tag{104}$$

$$z_2^{11} = \alpha z_2^{(2)}(0) , \tag{105}$$

$$z_1^{(4)}(T_4) = \beta z_1^{(2)}(0) , \tag{106}$$

$$z_2^{(4)}(T_4) = \beta z_2^{(2)}(0) . \tag{107}$$

Using Equation (11) and Equations (95) and (96), one has at the separating point

$$z_1^{(2)}(T_2) = z_1^{(3)}(0) + z_1^{(4)}(0) , \tag{108}$$

$$z_2^{(2)}(T_2) = z_2^{(3)}(0) + z_2^{(4)}(0) . \tag{109}$$

Since the objective function is $x_2^{(3)}(T_3)$

$$z_2^{(3)}(T_3) = c_2^{(3)} = 1 , \tag{110}$$

$$z_1^{(3)}(T_3) = c_1^{(3)} = 0 . \tag{111}$$

It is seen from Equation (103)

$$z_i^{(k)} = \text{constant} , \qquad \begin{array}{l} k = 3,\ 4 \\ i = 1,\ 2 . \end{array} \tag{112}$$

Combining Equations (108), (109), (110), (111), and (112) gives

$$z_1^{(2)}(T_2) = z_1^{(4)}(0) , \tag{113}$$

$$z_2^{(2)}(T_2) = 1 + z_2^{(4)}(0) . \tag{114}$$

Combining Equations (104), (105), (106), (107), (112), (113), and (114) gives

$$z_1^{(2)}(T_2) = z_1^{(4)}(0) = z_1^{(4)}(T_4) = \beta z_1^{(2)}(0) , \tag{115}$$

$$z_2^{(2)}(T_2) = 1 + z_2^{(4)}(0) = 1 + z_2^{(4)}(T_4) = 1 + \beta z_2^{(2)}(0) , \tag{116}$$

and

$$z_1^{(2)}(T_2) = \beta z_1^{(2)}(0) = \frac{\beta}{\alpha} z_1^{11} , \tag{117}$$

$$z_2^{(2)}(T_2) = 1 + \beta z_2^{(2)}(0) = 1 + \frac{\beta}{\alpha} z_2^{11} . \tag{118}$$

Equations (115), (116), (117), and (118) are the boundary conditions. Assuming that the maximum values of H^{11} and $H^{(2)}$ occur at the stationary points, one obtains the optimal $\bar{\theta}^{11}$ and $\bar{\theta}^{(2)}$ from the conditions

$$\frac{\partial H^{11}}{\partial \theta^{11}} = 0 \tag{119}$$

and

$$\frac{\partial H^{(2)}}{\partial \theta^{(2)}} = 0 . \tag{120}$$

Solving Equation (120) gives

$$\bar{\theta}^{(2)} = \frac{\dfrac{E_1 - E_2}{R}}{\ln \left\lfloor \eta \dfrac{x_1^{(2)}}{x_2^{(2)}} \left(\dfrac{z_2^{(2)} - z_1^{(2)}}{z_2^{(2)}} \right) \right\rfloor} , \qquad \eta = \frac{k_{10}E_1}{k_{20}E_2} . \tag{121}$$

Since it is difficult to solve Equation (119) for $\bar{\theta}^{11}$ explicitly, one shall define

$$z_1^{11} = - \left(\frac{\partial h_1}{\partial x_1^{11}} \tilde{z}_1^{11} + \frac{\partial h_2}{\partial x_1^{11}} \tilde{z}_2^{11}\right) , \tag{122}$$

$$z_2^{11} = - \left(\frac{\partial h_1}{\partial x_2^{11}} \tilde{z}_1^{11} + \frac{\partial h_2}{\partial x_2^{11}} \tilde{z}_2^{11}\right) , \tag{123}$$

where h_1 and h_2 are the implicit forms of Equations (83) and (89)

$$h_1(x_1^{11}, x_2^{11}, \theta^{11}) = 0 , \tag{124}$$

$$h_2(x_1^{11}, x_2^{11}, \theta^{11}) = 0 . \tag{125}$$

Differentiating Equations (124) and (125) with respect to θ^{11} gives

$$\frac{\partial h_1}{\partial \theta^{11}} + \frac{\partial h_1}{\partial x_1^{11}} \frac{\partial x_1^{11}}{\partial \theta^{11}} + \frac{\partial h_1}{\partial x_2^{11}} \frac{\partial x_2^{11}}{\partial \theta^{11}} = 0 , \tag{126}$$

$$\frac{\partial h_2}{\partial \theta^{11}} + \frac{\partial h_2}{\partial x_1^{11}} \frac{\partial x_1^{11}}{\partial \theta^{11}} + \frac{\partial h_2}{\partial x_2^{11}} \frac{\partial x_2^{11}}{\partial \theta^{11}} = 0 . \tag{127}$$

From Equation (119) one has

$$\frac{\partial H^{11}}{\partial \theta^{11}} = 0 = z_1^{11} \frac{\partial x_1^{11}}{\partial \theta^{11}} + z_2^{11} \frac{\partial x_2^{11}}{\partial \theta^{11}} . \tag{128}$$

Substituting Equations (122) and (123) into Equation (128) and making use of Equations (126) and (127), one obtains

$$\frac{\partial H^{11}}{\partial \theta^{11}} = 0 = \tilde{z}_1^{11} \frac{\partial h_1}{\partial \theta^{11}} + \tilde{z}_2^{11} \frac{\partial h_2}{\partial \theta^{11}} = 0 . \tag{129}$$

Solving Equation (129) for $\bar{\theta}^{11}$ yields

$$\bar{\theta}^{11} = \frac{\dfrac{E_1 - E_2}{R}}{\ln \left[\eta \dfrac{x_1^{11}}{x_2^{11}} \left(\dfrac{z_2^{11} - z_1^{11}}{z_2^{11}} \right) \right]} . \tag{130}$$

Since

$$x_2^{(3)}(T_3) = x_2^{(3)}(0) = x_2^{(2)}(T_2) .$$

The expression for the maximum yield is obtained by substituting Equation (121) into Equation (91)

$$\frac{dx_2^{(2)}}{dt} = k_{10} \ln \left[\eta \frac{x_1^{(2)}}{x_2^{(2)}} \left(\frac{z_2^{(2)} - z_1^{(2)}}{z_2^{(2)}} \right) \right]^{\lambda_1} x_1^{(2)}$$

$$- k_{20} \ln \left[\eta \frac{x_1^{(2)}}{x_2^{(2)}} \left(\frac{z_2^{(2)} - z_1^{(2)}}{z_2^{(2)}} \right) \right]^{\lambda_2} x_2^{(2)} .$$

where

$$\lambda_1 = \frac{E_1}{E_2 - E_1} \quad , \quad \lambda_2 = \frac{E_2}{E_2 - E_1}$$

IV. THE MAXIMUM PRINCIPLE AND THE VARIATIONAL TECHNIQUES

In preceding chapters the variational principle has been used to derive the various forms of the maximum principle. There are several other optimization methods and techniques which are based on the variational principle and related techniques. Two of the better known methods are the calculus of variations and dynamic programming.

In this chapter the interrelationships among the various methods together with some general aspects of the variational principle are discussed.

The Maximum Principle and the Calculus of Variations (10)

In this section the well-known fundamental necessary conditions in the calculus of variations are derived from the maximum principle when the decision vector is not constrained. Conversely, by using the calculus of variations techniques, the weakened form of the maximum principle can be derived. It is worth noting that the calculus of variations is often frustrated in solving problems when

a. there is linearity in the decision variables,

b. they are two-point boundary value problems,

c. there are unusual functions,

d. there are inequality constraints on the decision variables (11).*

1. <u>The fundamental problem of the calculus of variations</u>. The problem may be formulated as follows (15)

---

* There have been some successful attempts to extend the classical calculus of variations to the case where the decision variables are constrained (12, (13, 14).

A real function

$$F(t, x_1(t), x_2(t), \ldots, x_s(t); \theta_1(t), \theta_2(t), \ldots, \theta_s(t)) = F(t, x(t), \theta(t))$$

is defined in some region R of the space of the real variables t, x_1, $x_2, \ldots,$ x_s for arbitrary real finite values θ_1, $\theta_2, \ldots, \theta_s$. The function F is continuous in all its arguments. One shall consider the collection of all piece-wise smooth curves

$$\bar{x}_i = \bar{x}_i(t), \qquad i = 1, 2, \ldots, s, \qquad t_0 \leq t \leq T \,, \tag{1}$$

lying in the region R and joining the points

$$(t_0, x(0)) = (t_0, \alpha_1, \alpha_2, \ldots, \alpha_s) = (t \;, \alpha) \,, \tag{2}$$

and

$$(T, x(T)) = (T, \beta_1, \beta_2, \ldots, \beta_s) = (T, \beta) \,. \tag{3}$$

Along each such admissible comparison curve, the objective function in the form

$$S = \int_{t_0}^{T} F\ (t, x(t), \dot{x}(t))\ dt \tag{4}$$

has a well defined value.

The problem is to find the curve (or the extremal) such that the objective function has an extremum.

The functions

$$x\ (t), \qquad i = 1, 2, \ldots, s$$

are assumed to be absolutely continuous and to have bounded derivatives, that is, at every point where the derivative exists,

$$\frac{dx_i(t)}{dt} \leq M \text{ (constant)}, \qquad i = 1, 2, \ldots, s; \qquad t \;\leq t \leq T. \tag{5}$$

The set of all absolutely continuous curves

$$x = (x_1(t), x_2(t), \ldots, x_s(t)), \qquad t_0 \leq t \leq T$$

are in a δ-neighborhood of $\bar{x}_i(t)$ if

$$x_i(t) - \bar{x}_i(t) < \delta, \qquad \text{for } t_0 \leq t \leq T, \qquad i = 1, 2, \ldots, s$$

2. The Euler-Lagrange equation and Legendre's necessary condition. Consider the following specific set of differential equations

$$\dot{x}_i(t) = \frac{dx_i(t)}{dt} = \theta_i(t) \; , \qquad i = 1, 2, \ldots, s \tag{6}$$

and the objective function

$$S = \int_{t_0}^{T} F(t, x_1(t), x_2(t), \ldots, x_s(t); \theta_1(t), \theta_2(t), \ldots, \theta_s(t)) \, dt$$

$$= \int_{t_0}^{T} F(t, x(t), \theta(t)) \, dt$$

which is to be minimized or maximized.

Using Equation (6), one has

$$S = \int_{t_0}^{T} F(t, x(t), \dot{x}(t)) \, dt \; . \tag{7}$$

The decision vector $\theta(t)$, $t_0 \leq t \leq T$, which is assumed to be piece-wise continuous, and the corresponding absolutely continuous trajectory $x(t)$ of the system represented by Equation (6) together with the boundary conditions given by Equations (2) and (3), will be called optimal if there exists a $\delta > 0$ such that

$$S\left[x(t), \theta(t)\right] \geq S\left[\bar{x}(t), \bar{\theta}(t)\right] ,$$

or

$$S\left[x(t), \theta(t)\right] \leq S\left[\bar{x}(t), \bar{\theta}(t)\right]$$

for every decision $\theta(t)$ for which the corresponding trajectory $x(t)$ lies in

the δ-neighborhood of the curve $\bar{x}(t)$. In the former case the objective function attains its minimum and in the latter, the maximum.

Since the maximum principle is a necessary condition for optimality, it is at the same time a necessary condition for the curve $\bar{x}(t)$ to be an extremal of the objective function represented by Equation (7). The fundamental problem of the calculus of variations is the one in which final time is specified and both end points are fixed.

In order to obtain the Euler-Lagrange equation from the maximum principle, an additional state variable x_{s+1} is introduced such that

$$\dot{x}_{s+1}(t) = \frac{dx_{s+1}}{dt} = F(t,\ x(t),\ \theta(t)); \quad x_{s+1}(0) = 0 \ . \tag{8}$$

Thus the Hamiltonian and the adjoint system take the form

$$\begin{aligned} H &= \sum_{i=1}^{s+1} z_i\,\dot{x}_i \\ &= z_1\theta_1 + z_2\theta_2 + \dots + z_s\theta_s + z_{s+1}F \ , \end{aligned} \tag{9}$$

$$\frac{dz_i}{dt} = -\frac{\partial H}{\partial x_i} = -\ z_{s+1}\,\frac{\partial F(t,\ x,\ \theta)}{\partial x_i} \ , \qquad i = 1,\ 2, \dots,\ s \tag{10}$$

$$\frac{dz_{s+1}}{dt} = 0 \ . \tag{11}$$

Assuming that the optimum lies in the interior portion of the admissible region of $\theta(t)$, the optimal condition is determined from the following:

$$\frac{\partial H}{\partial \theta_i} = 0 = z_i + z_{s+1}\,\frac{\partial F(t,\ x,\ \theta)}{\partial \theta_i} \ , \qquad i = 1,\ 2, \dots,\ s \tag{12}$$

Since

$$z_{s+1}(T) = 1 \ .$$

From Equation (11) one thus has

$$z_{s+1}(t) = 1 \ . \tag{13}$$

Hence Equation (12) is reduced to

$$z_i(t) = -\frac{\partial F(t, x, \theta)}{\partial \theta_i} = -\frac{\partial F(t, x, \dot{x})}{\partial \dot{x}_i} . \qquad (14)$$

Substituting Equation (13) into Equation (10) and integrating the resulting equation give

$$z_i(t) = z_i(t_0) - \int_{t_0}^{T} \frac{\partial F(t, x, \theta)}{\partial x_i}\, dt, \qquad i = 1, 2, \ldots, s. \qquad (15)$$

Combining Equations (14) and (15), one obtains

$$\frac{\partial F(t, x, \theta)}{\partial \dot{x}_i} = \int_{t_0}^{T} \frac{\partial F(t, x, \theta)}{\partial x_i}\, dt - z_i(t_0), \qquad i = 1, 2, \ldots, s \qquad (16)$$

which are the Euler-Lagrange equations in the integral form. Differentiating Equation (16) with respect to t yields

$$\frac{\partial F(t, x, \theta)}{\partial x_i} - \frac{d}{dt}\left(\frac{\partial F(t, x, \theta)}{\partial \dot{x}_i}\right) = 0 , \qquad i = 1, 2, \ldots, s \qquad (17)$$

which are the Euler-Lagrange equations in the usual form.

In solving problems by using the calculus of variations, the existence and continuity of all partial derivatives of $F(t, x, \dot{x})$ up to the fourth order are assumed (16). Then, if the Hamiltonian attains its minimum as a function of $\theta(t)$, the quadratic form

$$\sum_{i=1}^{s} \sum_{j=1}^{s} \left.\frac{\partial^2 H(t, z(t), x(t), \theta(t))}{\partial \theta_i\, \partial \theta_j}\right|_{\theta = \bar{\theta}} \xi_i\, \xi_j \geq 0 .$$

It follows from Equations (9) and (13) that

$$\sum_{i=1}^{s} \sum_{j=1}^{s} \left.\frac{\partial^2 F(t, x(t), \theta(t))}{\partial \theta_i\, \partial \theta_j}\right|_{\theta = \bar{\theta}} \xi_i\, \xi_j \geq 0 \text{ for all } t,\ t_0 \leq t \leq T \qquad (18)$$

where ξ is an arbitrary constant. This condition which is necessary for the curve $x(t)$ to be an extremal for the minimum objective function, is called

Legendre's necessary condition.

3. Weierstrass necessary condition. According to the maximum principle the necessary condition for a minimum objective function is that

$$H(t, x(t), z(t), \theta(t)) \geq H(t, x(t), z(t), \bar{\theta}(t)) \ . \tag{19}$$

Using Equation (9), we consider

$$H(t, x(t), z(t), \theta(t)) - H(t, x(t), z(t), \bar{\theta}(t))$$

$$- \sum_{i=1}^{s} (\theta_i - \bar{\theta}_i) \frac{\partial H(t, x(t), z(t), \bar{\theta}(t))}{\partial \bar{\theta}_i}$$

$$= z_{s+1} \left[F(t, x, \theta) - F(t, x, \bar{\theta}) \right] + \sum_{i=1}^{s} z_i (\theta_i - \bar{\theta}_i)$$

$$- \sum_{i=1}^{s} (\theta_i - \bar{\theta}_i) \left[\frac{\partial F(t, x, \bar{\theta})}{\partial \bar{\theta}_i} z_{s+1} + z_i \right]$$

$$= z_{s+1} \left\{ \left[F(t,x,\theta) - F(t,x,\bar{\theta}) \right] - \sum_{i=1}^{s} (\theta_i - \bar{\theta}_i) \frac{\partial F(t, x, \bar{\theta})}{\partial \bar{\theta}_i} \right\} \tag{20}$$

Substituting Equation (13) into Equation (20) gives

$$H(t, x, z, \theta) - H(t, x, z, \bar{\theta}) - \sum_{i=1}^{s} (\theta_i - \bar{\theta}_i) \frac{\partial H(t, x, z, \bar{\theta})}{\partial \bar{\theta}_i}$$

$$= \left\{ \left[F(t, x, \theta) - F(t, x, \bar{\theta}) \right] - \sum_{i=1}^{s} (\theta_i - \bar{\theta}_i) \frac{\partial F(t, x, \bar{\theta})}{\partial \bar{\theta}_i} \right\} . \tag{21}$$

In the calculus of variations the Weierstrass E-function is defined as

$$E = F(t, x, \theta) - F(t, x, \bar{\theta}) - \sum_{i=1}^{s} (\theta_i - \bar{\theta}_i) \frac{\partial F(t, x, \bar{\theta})}{\partial \bar{\theta}_i} \ . \tag{22}$$

If the Hamiltonian function attains its maximum at an interior point of the region in which the decision vector $\theta(t)$ (or $\dot{x}(t)$) is defined, one has

$$\frac{\partial H(t, x, z, \bar{\theta})}{\partial \bar{\theta}_i} = 0 \ , \qquad i = 1, 2, \ldots, s. \tag{23}$$

Combination of Equations (19), (21), (22), and (23) yields

$$E \geq 0 , \tag{24}$$

which is the Weierstrass necessary condition for a minimum objective function. It is worth noting that Equation (24) is not applicable if the decision vector $\theta(t)$ lies on the boundary of the region defined. However, the maximum principle does not have this deficiency (10).

4. The problem of Bolza. The problem of Bolza as formulated by Bliss (16) is stated as follows:

It is desired to find in a class of curves

$$x_i(t) , \qquad i = 1, 2, \ldots, s, \qquad t_0 \leq t \leq T$$

satisfying the differential equations

$$\Phi_j(t, x(t), \dot{x}(t)) = 0, \qquad j = 1, 2, \ldots, m < s \tag{25}$$

and the end conditions

$$\psi_k(t_0, x(t_0), T, x(T)) = 0, \qquad k = 1, 2, \ldots, p \leq 2s + 2 \tag{26}$$

a curve which minimizes an objective function of the form

$$S = g\left[t_0, x(t_0), T, x(T)\right] + \int_{t_0}^{T} F(t, x(t), \dot{x}(t))\, dt . \tag{27}$$

It will be shown that the optimization problem which has been treated so far is equivalent to the problem of Bolza in which either $g = 0$ or $F = 0$, that is, it is equivalent to the problem of Lagrange or the problem of Mayer.

Consider the following system of differential equations

$$\frac{dx_i}{dt} = f_i(t, x_1(t), x_2(t), \ldots, x_s(t), \frac{dx_{m+1}}{dt}, \ldots, \frac{dx_s}{dt}) , \tag{28}$$

$$i = 1, 2, \ldots, m < s$$

and

$$\frac{dx_{m+j}}{dt} = \theta_j, \qquad j = 1, 2, \ldots, s-m. \tag{29}$$

Equation (28) can be rewritten as

$$\frac{dx_i}{dt} - f_i(t,\ x_1(t),\ x_2(t), \ldots,\ x_s(t),\ \frac{dx_{m+1}}{dt},\ \ldots,\ \frac{dx_s}{dt})$$

$$= \Phi_i(t,\ x_1(t), \ldots,\ x_s(t),\ \frac{dx_{m+1}}{dt}, \ldots,\ \frac{dx_s}{dt}) = 0\ , \qquad (30)$$

$$i = 1,\ 2, \ldots,\ m < s.$$

This is equivalent to Equation (25).

The boundary conditions of the optimization problem are usually of the form

$$x(t_0) = \alpha\ , \qquad x(T) = \beta \qquad (31)$$

which is equivalent to Equation (26). The problem is to find an admissible optimal control (or the optimal decision) $\theta(t)$ such that the corresponding trajectory of the system satisfies Equations (30) and (31) and that the objective function

$$S = \int_{t_0}^{T} F(t,\ x(t),\ \theta(t))\ dt,$$

which can be obtained from Equation (27) by setting

$$g = 0\ ,$$

attains its minimum. It may be noted that the problem in which the objective function is of the form

$$S = \sum_{i=1}^{s} c_i\ x_i(T)$$

has also been treated before. This is equibalent to the case

$$F = 0$$

in Equation (27). The values of t_0 and $x(t_0)$ are usually given. $x(T)$ is to be determined and T may be fixed or unspecified. It may also be noted that

problems in which the objective function is in the integral form can be reduced to the form of the linear combination of the final state variable by introducing an additional state variable.

5. From the calculus of variations to the maximum principle. The maximum principle can be derived by using the classical calculus of variations, if the decision variables are not constrained.

Suppose that a piece-wise smooth curve

$$x = \bar{x}(t), \qquad t_0 \leq t \leq T$$

lies entirely in the space of the real variables $t, x_1, x_2, \ldots, x_s$ and gives the objective function S a weak relative extremum. A piece-wise smooth vector function

$$y(t) = (y_1(t), y_2(t), \ldots, y_s(t))$$

is chosen such that it satisfies the boundary conditions

$$y_i(t_0) = 0, \qquad i = 1, 2, \ldots, s. \tag{32}$$

Consider the equation

$$x(t) = \bar{x}(t) + \epsilon y(t) . \tag{33}$$

If ϵ is sufficiently small, the function $x(t)$ lies in a neighborhood of the extremal $\bar{x}(t)$. The corresponding equation for $\theta(t)$ is

$$\theta(t) = \bar{\theta}(t) + \epsilon\varphi(t). \tag{34}$$

Then the objective function can be considered as a function of ϵ, that is

$$S(\bar{x}(t) + \epsilon y(t)) = \psi(\epsilon), \tag{35}$$

and it attains its extremum when $\epsilon = 0$. Consequently, the condition

$$\psi'(0) = \frac{d\psi}{d\epsilon}\bigg|_{\epsilon=0} = 0 \tag{36}$$

provides the necessary condition for the extremum. The objective function which is to be minimized is of the form

$$S = \sum_{i=1}^{s} c_i \, x_i(T). \tag{37}$$

It can be written in the form

$$S = \int_{t_0}^{T} \sum_{i=1}^{s} c_i \, \dot{x}_i \, dt + \sum_{i=1}^{s} c_i \, x_i(t_0). \tag{38}$$

The performance equations are

$$\frac{dx_i}{dt} = \dot{x}_i(t) = f_i(t, x(t), \theta(t)), \qquad i = 1, 2, \ldots, s \tag{39}$$

or

$$\dot{x}_i(t) - f_i(t, x(t), \theta(t)) = 0, \qquad i = 1, 2, \ldots, s. \tag{40}$$

Employing $-z_i(t)$ as the Lagrange multipliers, one has

$$S = \int_{t_0}^{T} \left[\sum_{i=1}^{s} c_i \dot{x}_i - \sum_{i=1}^{s} z_i(t)(\dot{x}_i(t) - f_i(t, x(t), \theta(t)) \right] dt$$
$$+ \sum_{i=1}^{s} c_i \, x_i(t_0). \tag{41}$$

Differentiating the above equation with respect to ϵ gives

$$\psi'(0) = 0 = \int_{t_0}^{T} \left[\sum_{i=1}^{s} (c_i - z_i(t)) \frac{dy_i(t)}{dt} - \sum_{i=1}^{s} \sum_{j=1}^{s} z_i(t) \frac{\partial f_i(t, \bar{x}, \bar{\theta})}{\partial \bar{x}_j} y_j \right] dt$$
$$- \int_{t_0}^{T} \left[\sum_{i=1}^{s} \sum_{j=1}^{r} z_i \frac{\partial f_i(t, \bar{x}, \bar{\theta})}{\partial \bar{\theta}_j} \varphi_j \right] dt = 0 \; , \tag{42}$$

where r is the number of components of the decision vector.

Integrating by parts the first term in the first bracketed quantity on the right hand side of Equation (42), one obtains

$$- \left[\sum_{i=1}^{s} (c_i - z_i(t)) y_i(t) \right]_{t_0}^{T} = \int_{t_0}^{T} \left[\sum_{i=1}^{s} \frac{dz_i(t)}{dt} + \sum_{i=1}^{s} \sum_{j=1}^{s} z_j(t) \frac{\partial f_j(t, \bar{x}, \bar{\theta})}{\partial \bar{x}_i} \right] y_i \, dt$$

$$+\int_{t_0}^{T} \sum_{i=1}^{s} \sum_{j=1}^{r} z_i(t) \frac{\partial f_i(t, \bar{x}, \bar{\theta})}{\partial \bar{\theta}_j} \varphi_j \, dt. \tag{43}$$

Applying the boundary conditions, Equation (32), to Equation (43) gives

$$-\left[\sum_{i=1}^{s} (c_i - z_i(T)) y_i(T)\right] = \int_{t_0}^{T} \left[\sum_{i=1}^{s} \frac{dz_i(t)}{dt} + \sum_{i=1}^{s} \sum_{j=1}^{s} z_j(t) \frac{\partial f_j(t, \bar{x}(t), \bar{\theta}(t))}{\partial \bar{x}_i}\right] y_i(t) dt$$

$$+\int_{t_0}^{T} \sum_{i=1}^{s} \sum_{j=1}^{r} z_i(t) \frac{\partial f_i(t, \bar{x}(t), \bar{\theta}(t))}{\partial \bar{\theta}_j} \varphi_j \, dt. \tag{44}$$

Since $y_i(t)$ and $\varphi_j(t)$ are arbitrary on the interval $t_0 \leq t \leq T$, in order for Equation (44) to be an equality, the following conditions must be satisfied

$$\left.\begin{aligned} &c_i - z_i(T) = 0 , \\ &\frac{dz_i(t)}{dt} + \sum_{j=1}^{s} z_j(t) \frac{\partial f_j(t, \bar{x}(t), \bar{\theta}(t))}{\partial \bar{x}_i} = 0, \end{aligned}\right\} \quad i = 1, 2, \ldots, s \tag{45}$$

and

$$\sum_{i=1}^{s} z_i(t) \frac{\partial f_j(t, \bar{x}(t), \bar{\theta}(t))}{\partial \bar{\theta}_j} = 0 , \qquad j = 1, 2, \ldots, r \tag{46}$$

or

$$z_i(T) = c_i , \qquad i = 1, 2, \ldots, s \tag{47}$$

$$\frac{dz_i}{dt} = -\sum_{j=1}^{s} z_j(t) \frac{\partial f_j(t, \bar{x}(t), \bar{\theta}(t))}{\partial \bar{x}_i} , \quad i = 1, 2, \ldots, s \tag{48}$$

and

$$\sum_{i=1}^{s} z_i \frac{\partial f_i(t, \bar{x}(t), \bar{\theta}(t))}{\partial \theta_j} , \qquad j = 1, 2, \ldots, r. \tag{49}$$

Equations (47) and (48) are the adjoint system in the maximum principle and Equation (49) is the necessary condition for the extremum. It is noted that the derivation used in this section leads only to the stationary condition

of the maximum principle (18).

6. <u>The canonical equations and transformations</u>. There are many different ways by which coordinates can be transformed. In general the objective of a transformation is to change an original system of equations to a new system of equivalent equations such that the latter system is easier to handle and clearer to visualize than the original form. The transformation which has been used is equivalent to the one frequently applied in the classical mechanics. In this section a transformation which leads to the algorithm of the maximum principle is presented.

Suppose that an objective function of the form

$$S = \int_{t_0}^{T} F(t,\ x(t),\ \theta(t))\ dt$$

is to be minimized, where

$$\theta_i(t) = \frac{dx_i}{dt} = \dot{x}_i(t)\ , \qquad i = 1,\ 2, \ldots,\ s.$$

Define the Hamiltonian function and the adjoint variables as follows: (19):

$$H = \sum_{i=1}^{s} z_i\ \dot{x}_i + z_{s+1}\ F(t,\ x(t),\ \theta(t))$$

$$= \sum_{i=1}^{s} z_i\ \dot{x}_i + F(t,\ x(t),\ \theta(t)). \tag{50}$$

and

$$z_i(t) = -\frac{\partial F}{\partial \dot{x}_i}\ , \qquad i = 1,\ 2, \ldots,\ s. \tag{51}$$

Assuming that the Jacobian

$$\frac{\partial\ (z_1,\ z_2, \ldots,\ z_s)}{\partial\ (\dot{x}_1,\ \dot{x}_2, \ldots,\ \dot{x}_s)} \neq 0\ .$$

we can make a local transformation from the variables t, $x_1, x_2, \ldots, x_s$, $\dot{x}_1, \dot{x}_2, \ldots, \dot{x}_s$, F to the variables t, $x_1, x_2, \ldots, x_s$, $z_1, z_2, \ldots, z_s$, H, which are called canonical variables.

Hence the Hamiltonian and adjoint system of the maximum principle can be derived by using the definitions of Equations (50) and (51). From Equation (50) one has

$$dH = \sum_{i=1}^{s} z_i \, d\dot{x}_i + \sum_{i=1}^{s} \dot{x}_i \, dz_i + \frac{\partial F}{\partial t} dt + \sum_{i=1}^{s} \frac{\partial F}{\partial x_i} dx_i + \sum_{i=1}^{s} \frac{\partial F}{\partial \dot{x}_i} d\dot{x}_i . \qquad (52)$$

Substituting Equation (51) into Equation (52) gives

$$dH = \sum_{i=1}^{s} \dot{x}_i \, dz_i + \frac{\partial F}{\partial t} dt + \sum_{i=1}^{s} \frac{\partial F}{\partial x_i} dx_i . \qquad (53)$$

It follows from Equation (53) that

$$\frac{\partial H}{\partial t} = \frac{\partial F}{\partial t} , \qquad (54)$$

$$\frac{\partial H}{\partial x_i} = \frac{\partial F}{\partial x_i} , \qquad (55)$$

$$i = 1, 2, \ldots, s$$

$$\frac{\partial H}{\partial z_i} = \dot{x}_i = \frac{dx_i}{dt} . \qquad (56)$$

The Euler-Lagrange equations for the objective function S are

$$\frac{\partial F}{\partial x_i} - \frac{d}{dt} \frac{\partial F}{\partial \dot{x}_i} = 0 , \qquad i = 1, 2, \ldots, s. \qquad (57)$$

Combining Equations (51), (55), (56), and (57) gives the following set of equations called the canonical Euler equations (19)

$$\frac{dz_i}{dt} = - \frac{\partial H}{\partial x_i} , \qquad (58)$$

$$i = 1, 2, \ldots, s$$

$$\frac{dx_i}{dt} = \frac{\partial H}{\partial z_i} , \qquad (59)$$

If the Hamiltonian function does not depend on t explicitly, we have

$$\frac{dH}{dt} = \sum_{i=1}^{s} \left(\frac{\partial H}{\partial x_i}\frac{dx_i}{dt} + \frac{\partial H}{\partial z_i}\frac{dz_i}{dt}\right) . \tag{60}$$

Substituting Equations (58) and (59) into Equation (60) yields

$$\frac{dH}{dt} = \sum_{i=1}^{s} \left(\frac{\partial H}{\partial x_i}\frac{\partial H}{\partial z_i} - \frac{\partial H}{\partial x_i}\frac{\partial H}{\partial z_i}\right) = 0. \tag{61}$$

Therefore, it follows that H is constant along the extremal.

The transformation from the variables t, x, $\dot{x}$, and the function $F(t, x, \dot{x})$ to those of t, x, z, and $H(t, x, z)$ respectively is called the Legendre transformation (19). If $H(t, x, z)$ is subjected to the Legendre transformation, the function F is recovered as follows:

Using Equations (50) and (56), we have

$$H - \sum_{i=1}^{s} z_i \frac{\partial H}{\partial z_i} = \sum_{i=1}^{s} z_i \dot{x}_i + F(t, x(t), \dot{x}(t)) - \sum_{i=1}^{s} z_i \dot{x}_i$$
$$= F(t, x(t), \dot{x}(t)).$$

This indicates that the Legendre transformation is its own inverse.

7. <u>The transversality conditions</u>. Suppose that the objective function is of the form

$$S = \int_{t_0}^{T} F(t, x(t), \dot{x}(t))\, dt , \tag{62}$$

and that the initial point is fixed at

$$x(t_0) = \alpha ,$$

and that the final point lies on the given hypersurface

$$h(x(T)) = 0. \tag{63}$$

Let $\bar{T}$ be the final time when the optimal trajectory hits the given surface. One then has

$$T = \bar{T} + \delta T ,$$

and the variational equation is

$$x(t) = \bar{x}(t) + \epsilon y(t). \tag{64}$$

The difference of the objective function is

$$\Delta S = \int_{t_0}^{\bar{T}+\delta T} F(t,\ x+\epsilon y,\ \dot{x}+\epsilon\dot{y})\ dt - \int_{t_0}^{\bar{T}} F(t,\ x,\ \dot{x})\ dt$$

$$= \int_{t_0}^{\bar{T}} \Big[F(t,\ x+\epsilon y,\ \dot{x}+\epsilon\dot{y}) - F(t,\ x,\ \dot{x})\Big]\ dt$$

$$+ \int_{\bar{T}}^{\bar{T}+\delta T} F(t,\ x+\epsilon y,\ \dot{x}+\epsilon\dot{y})\ dt\ . \tag{65}$$

Hence the variation of the objective function becomes

$$\delta S = \int_{t_0}^{\bar{T}} \sum_{i=1}^{s} \left(\frac{\partial F}{\partial x_i}\ \epsilon y_i + \frac{\partial F}{\partial \dot{x}_i}\ \epsilon\dot{y}_i\right) dt + F\Big|_{t=\bar{T}} \delta T. \tag{66*}$$

Integrating the second member of the first term in Equation (66) by parts gives

$$\delta S = \int_{t_0}^{\bar{T}} \sum_{i=1}^{s} \left(\frac{\partial F}{\partial x_i} - \frac{d}{dt}\frac{\partial F}{\partial \dot{x}_i}\right) \epsilon y_i(t)\ dt + \sum_{i=1}^{s} \frac{\partial F}{\partial \dot{x}_i}\ \epsilon y_i(t)\Big|_{t_0}^{\bar{T}} + F\Big|_{t=\bar{T}} \delta T. \tag{67}$$

It can be seen from Figure 8 that

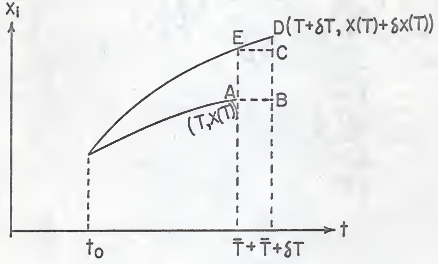
$$\epsilon y_i(t)\ \Big|_{t=\bar{T}} \doteq \delta x_i(T) - \dot{x}_i(T)\ \delta T. \tag{68}$$

Substituting Equation (68) into Equation (67) yields

$$\delta S = \int_{t_0}^{\bar{T}} \sum_{i=1}^{s} \left(\frac{\partial F}{\partial x_i} - \frac{d}{dt}\frac{\partial F}{\partial \dot{x}_i}\right)\epsilon y_i(t)\ dt + \left(F - \sum_{i=1}^{s} \dot{x}_i \frac{\partial F}{\partial \dot{x}_i}\right) \delta t\ \Big|_{t=\bar{T}}$$

---

* $\frac{d}{dt}\Big[\epsilon y(t)\Big] = \epsilon\dot{y}(t)$, that is, the derivative of a variation is the variation of a derivative (17).



$AE = \epsilon y_i(T)\big|_{t=T}$ $\quad BD = \delta x_i(T)$

$CD \doteq \dot{x}_i(T)\,\delta T$ $\quad AE = BD - CD$

Fig.8. Variation of the trajectory.

$$+ \sum_{i=1}^{s} \frac{\partial F}{\partial \dot{x}_i} \delta x_i \Big|_{t = \bar{T}} . \tag{69}$$

Since the objective function S has an extremum along the extremal $\bar{x}(t)$, the Euler-Lagrange equation must be satisfied, that is

$$\frac{\partial F}{\partial x_i} - \frac{d}{dt} \frac{\partial F}{\partial \dot{x}_i} = 0 , \qquad i = 1, 2, \ldots, s.$$

It follows that

$$\delta S = (F - \sum_{i=1}^{s} \dot{x} \frac{\partial F}{\partial \dot{x}_i}) \delta t \Big|_{t=\bar{T}} + \sum_{i=1}^{s} \frac{\partial F}{\partial \dot{x}_i} \delta x \Big|_{t=\bar{T}} . \tag{70}$$

Substituting Equations (50) and (51) into Equation (70), one obtains

$$\delta S = (\sum_{i=1}^{s} z_i \delta x_i - H \delta t) \Big|_{t=\bar{T}} . \tag{71}$$

Thus the necessary condition for an extremum

$$\delta S = 0$$

takes the form

$$\sum_{i=1}^{s} z_i \delta x_i - H \delta t = 0, \tag{72}$$

at $t = \bar{T}$. According to the theorem of Pontryagin for final time unspecified (see Appendix 1), if S attains a minimum

$$H_{min} = 0.$$

Equation (72) then becomes

$$\sum_{i=1}^{s} z_i \delta x_i = 0 , \tag{73}$$

at $t = \bar{T}$.

If the vector $a = (a_1, a_2, \ldots, a_s)$ belongs to the tangent plane of $h(x) = 0$ at $t = \bar{T}$, Equation (73) can be written as

$$\sum_{i=1}^{s} z_i \, a_i = 0. \tag{74}$$

Similarly, if the initial point $x(t_0)$ lies on the hypersurface

$$h(x(t_0)) = 0,$$

one can obtain the similar transversality condition

$$\sum_{i=1}^{s} z_i \, a_i = 0,$$

at $t = t_0$.

8. The Hamiltonian-Jacobi equation (19). If in Equation (71), one defines a new function

$$dW = \sum_{i=1}^{s} z_i \, dx_i - H \, dt \tag{75}$$

at $t = \bar{T}$, then it follows that

$$\frac{\partial W}{\partial x_i} = z_i, \qquad i = 1, 2, \ldots, s \tag{76}$$

$$\frac{\partial W}{\partial t} = - H. \tag{77}$$

From Equation (77), one has

$$\frac{\partial W}{\partial t} + H(t, x(t), \frac{\partial W}{\partial x_i}) = 0 \tag{78}$$

at $t = \bar{T}$. Equation (78) is known as the Hamiltonian-Jacobi equation. Let

$$W = W(t, x(t), \eta) \tag{79}$$

be a solution of the Hamiltonian-Jacobi equation, where

$\eta = (\eta_1, \eta_2, \ldots, \eta_m)$, $m \leq s$ is a parameter.

Then

$$\frac{d}{dt} \left(\frac{\partial W}{\partial \eta_i}\right) = 0, \qquad i = 1, 2, \ldots, m. \tag{80}$$

This can be shown as follows:

Since one has

$$\frac{d}{dt}\left(\frac{\partial W}{\partial \eta_i}\right) = \frac{\partial^2 W}{\partial t \ \partial \eta_i} + \sum_{j=1}^{s} \frac{\partial^2 W}{\partial x_j \, \partial \eta_i} \frac{dx_j}{dt} . \tag{81}$$

Substituting Equation (79) into Equation (78) and differentiating it with respect to η_i give

$$\frac{\partial^2 W}{\partial t \ \partial \eta_i} + \sum_{j=1}^{s} \frac{\partial H}{\partial z_i} \frac{\partial^2 W}{\partial x_j \, \partial \eta_i} = 0. \tag{82}$$

From Equations (81) and (82) one thus obtains

$$\begin{aligned} \frac{d}{dt}\left(\frac{\partial W}{\partial \eta_i}\right) &= \sum_{j=1}^{s} \frac{\partial H}{\partial z_j} \frac{\partial^2 W}{\partial x_j \, \partial \eta_i} - \sum_{j=1}^{s} \frac{\partial^2 W}{\partial x_j \, \partial \eta_i} \frac{dx_j}{dt} \\ &= \sum_{j=1}^{s} \frac{\partial^2 W}{\partial x_j \, \partial \eta_i} \left[\frac{\partial H}{\partial z_j} - \frac{dx_j}{dt}\right] = 0 . \end{aligned} \tag{83}$$

along each extremal. Comparing Equations (61) with Equation (83), one sets that both H and $\frac{\partial W}{\partial \eta_i}$ are the first integrals of the canonical Euler equations.

The Maximum Principle and Dynamic Programming

It will be shown in this section that there exists a close relation between the maximum principle and the method of dynamic programming.

The method of dynamic programming is based on the principle of optimality stated by Bellman (1) as

> "An optimal policy has the property that whatever the initial state and initial decision are, the remaining decisions must constitute an optimal policy with regard to the state resulting from the first decision."

It is desired to minimize an objective function of the form

$$S = \sum_{i=1}^{s} c_i \, x_i(T),$$

with the initial condition

$$x(t_0) = \alpha,$$

and with the final time T fixed.

The principle of optimality implicitly states that the minimum value of S is a function of the initial state $x(t_0) = \alpha$, and the initial time t_0. Introducing the function (20)

$$S(x(t_0),\, t_0) = \underset{\theta(t)}{\mathrm{Min}}\; S = \underset{\theta(t)}{\mathrm{Min}} \sum_{i=1}^{s} c_i \, x_i(T), \qquad t_0 \leq t \tag{84}$$

and denoting the optimal trajectory at $t = t_0 + \Delta t$ by $\bar{x}(t)$, where Δt is sufficiently small, one has

$$S(x(t_0),\, t_0) = S(\bar{x},\, t). \tag{85}$$

Assume that the trajectory from $t_0 + \Delta t$ to T is optimal. Then for any other trajectory $x(t)$ at $t_0 + \Delta t$, we have $S(x, t)$. From the definition of Equation (84), it follows that

$$S(x(t_0),\, t_0) = \underset{\theta(t)}{\mathrm{Min}}\; S(x,\, t), \qquad t_0 \leq t \leq t_0 + \Delta t. \tag{86}$$

Assuming the existence and continuity of the partial derivatives of $S(x, t)$, it can be expanded in a Taylor series to give

$$S(x,\, t) = S(x(t_0),\, t_0) + \sum_{i=1}^{s} \frac{\partial S}{\partial x_i} (x_i - x_i(t_0)) + \frac{\partial S}{\partial t_0} (t - t_0) + 0(\epsilon^2), \tag{87}$$

where the partial derivatives are evaluated at $(x(t_0), t_0)$, and $0(\epsilon^2)$ represents the terms of ϵ^2 and those of higher orders than ϵ^2. $0(\epsilon^2)$ should satisfy the condition that

$$\lim_{\Delta t \to 0} \frac{0(\epsilon^2)}{\Delta t} = 0.$$

The performance equations are again given by

$$\dot{x}_i(t) = \frac{dx_i}{dt} = f_i(t, x(t), \theta(t)), \qquad i = 1, 2, \ldots, s. \tag{88}$$

Hence

$$x_i(t) = x_i(t_0) + f_i(t_0, x(t_0), \theta(t_0))\,\Delta t + O(\epsilon^2). \tag{89}$$

Substituting Equations (87) and (89) into Equation (86) gives

$$S(x(t_0), t_0) = \underset{\theta(t)}{\text{Min}} \Big\lfloor S(x(t_0), t_0) + \sum_{i=1}^{s} \frac{\partial S}{\partial x_i} f_i\,\Delta t$$

$$+ \frac{\partial S}{\partial t_0}\Delta t + O(\epsilon^2)\Big\rfloor, \qquad t_0 \leq t \leq t_0 + \Delta t. \tag{90}$$

The decision vector consists of those terms containing f_i. By simplifying Equation (90) and dividing it by Δt, one obtains

$$\frac{\partial S(x(t_0), t_0)}{\partial t_0} = -\underset{\theta(t)}{\text{Min}} \Big\lfloor \sum_{i=1}^{s} \frac{\partial S}{\partial x_i} f_i + \frac{O(\epsilon^2)}{\Delta t}\Big\rfloor, \qquad t_0 \leq t \leq t_0 + \Delta t$$

Letting Δt approaches zero yields

$$\frac{\partial S(x(t_0), t_0)}{\partial t_0} = -\underset{\theta(t)}{\text{Min}} \sum_{i=1}^{s} \frac{\partial S}{\partial x_i} f_i\,(t_0, x(t_0), \theta(t_0)), \tag{91}$$

at $t = t_0$. This determines the choice of $\theta(t)$ at $t = t_0$. Equation (91) is valid for any t_0; it can be applied to any point in the interval $\lfloor t_0, T\rfloor$. Therefore, it can be written in general as

$$\frac{\partial S(x(t), t)}{\partial t} = -\underset{\theta(t)}{\text{Min}} \sum_{i=1}^{s} \frac{\partial S}{\partial x_i} f_i(t, x(t), \theta(t)). \tag{92}$$

It will be shown that this is equivalent to the optimal condition given by the maximum principle. Let

$$z_i(t) = -\frac{\partial S(x(t), t)}{\partial x_i}, \quad z(T) = c_i, \qquad i = 1, 2, \ldots, s \tag{93}$$

and

$$\frac{\partial S(x(t),\ t)}{\partial t} = H(t,\ \bar{x}(t),\ \bar{\theta}(t),\ z(t))$$

$$= \sum_{i=1}^{s} z_i(t)\ f_i(t,\ \bar{x}(t),\ \bar{\theta}(t)). \tag{94}$$

From Equations (93) and (94) one has

$$\frac{dz_i}{dt} = -\sum_{j=1}^{s} z_j \frac{\partial f_j}{\partial x_i} \tag{95}$$

then combining Equations (92), (93), and (94) one obtains

$$H(t,\ \bar{x}(t),\ \bar{\theta}(t),\ z(t)) = \underset{\theta(t)}{\mathrm{Min}}\ H(t,\ x(t),\ \theta(t),\ z(t)). \tag{96}$$

The relationship between the maximum principle and dynamic programming is analogous to that between the Hamiltonian system and the Hamiltonian-Jacobi equation [compare Equations (93), (94), and (96) with Equations (76), (77), and (78)].

Generally, in order to find the optimal trajectory, the method of dynamic programming requires the exhaustive stepwise calculation by using Equations (88) and (91), and the objective function

$$S = \sum_{i=1}^{s} c_i\ x_i(T).$$

However, using the technique of the maximum principle, one needs the solution of the differential equations, Equations (88) and (96), and the optimal condition, Equation (96). The advantages and the shortcomings of each method have been broadly discussed elsewhere (10, 11, 6, 21).

It is worthwhile to mention that the method of dynamic programming results in a set of partial differential equations, whereas the maximum principle gives a set of ordinary differential equations. The method of characteristics, however, can be used to transform the set of partial

differential equations to a set of ordinary differential equations (11).

Dynamic Programming and the Calculus of Variations

In the calculus of variations, we consider the properties of the admissible curves lying in the δ-neighborhood of the optimal curve and hence obtain all the necessary conditions. By using the method of dynamic programming, instead of finding the whole extremal, one evaluates the optimal derivative point by point along the extremal. It will be shown how the working equations of the calculus of variations can be derived by using dynamic programming.

Consider

$$\frac{dx_i}{dt} = \dot{x}_i(t) = \theta_i(t), \qquad i = 1, 2, \ldots, s. \tag{97}$$

It is desired to maximize the objective function S of the form

$$S = \int_{t_0}^{T} F(t, x(t), \dot{x}(t))\, dt.$$

The boundary conditions are

$$x(t_0) = \alpha ,$$
$$x(T) = \beta.$$

Define the function

$$S(t, x(t)) = \underset{\theta(t)}{\mathrm{Min}} \int_{t}^{T} F(t, x(t), \theta(t))\, dt , \tag{98}$$

where $S(t, x(t))$ is the minimum value of the integral of $F(t, x(t), \theta(t))$ from the point $(t, x(t))$ to the fixed point $(T, x(T))$. It is clear that

$$S(T, x(T)) = 0.$$

Breaking up the time interval $\lfloor t, T \rfloor$ into two parts, $\lfloor t, t+\Delta t \rfloor$ and

$\left[t+\Delta t,\ T\right]$, Equation (98) can be written as

$$S(t,\ x(t)) = \underset{\substack{\theta(t) \\ t\le t'\le t+\Delta t}}{\text{Min}} \quad \underset{\substack{\theta(t) \\ t+\Delta t\le t'\le T}}{\text{Min}} \left[\int_{t}^{t+\Delta t} F(t',\ x(t'),\ \theta(t'))\ dt' \right.$$

$$\left. + \int_{t+\Delta t}^{T} F(t',\ x(t'),\ \theta(t'))\right] dt'$$

$$= \underset{\substack{\theta(t) \\ t\le t'\le t+\Delta t}}{\text{Min}} \left[\int_{t}^{t+\Delta t} F(t',\ x(t'),\ \theta(t'))\ dt' \right.$$

$$\left. + \underset{\substack{\theta(t) \\ t+\Delta t\le t'\le T}}{\text{Min}} \int_{t+\Delta t}^{T} F(t',\ x(t'),\ \theta(t'))\ dt\right] . \qquad (99)$$

According to the definition given by Equation (98), one has

$$S(t+\Delta t,\ \dot{x}+x\Delta t) = \underset{\substack{\theta(t) \\ t+\Delta t\le t'\le T}}{\text{Min}} \int_{t+\Delta t}^{T} F(t',\ x(t'),\ \theta(t'))\ dt' .$$

Substituting this equation into Equation (99) gives

$$S(t,\ x(t)) = \underset{\substack{\theta(t) \\ t\le t'\le t+\Delta t}}{\text{Min}} \int_{t}^{t+\Delta t} F(t',\ x(t'),\ \theta(t'))\ dt' + S(t+\Delta t,\ x+\dot{x}\Delta t). \qquad (100).$$

For sufficiently small Δt, Equation (100) becomes

$$S(t,\ x(t)) = \underset{\substack{\theta(t) \\ t\le t'\le t+\Delta t}}{\text{Min}} \left[F(t,\ x(t),\ \theta(t))\Delta t + S(t+\Delta t,\ x+\dot{x}\Delta t)\right] + \left[O(\Delta t^2)\right] \qquad (101)$$

which is the functional formulation of the principle of optimality.

A Taylor series expansion of Equation (101) yields

$$S(t,\ x(t)) = \underset{\substack{\theta(t) \\ t\le t\le t+\Delta t}}{\text{Min}} \left[F(t,\ x(t),\ \theta(t))\ \Delta t + S(t,\ x(t))\right.$$

$$+ \frac{\partial S}{\partial t} \Delta t + \sum_{i=1}^{s} \frac{\partial S}{\partial x_i} \dot{x}_i \, \Delta t \Big] + 0(\Delta t^2). \quad (102)$$

Letting Δt approaches zero, the following nonlinear partial differential equation is obtained (22):

$$0 = \underset{\theta(t)}{\text{Min}} \left[F(t, x(t), \theta(t)) + \frac{\partial S}{\partial t} + \sum_{i=1}^{s} \dot{x}_i \frac{\partial S}{\partial x_i} \right] \quad (103)$$

which is an equation of the Hamiltonian-Jacpbi type and is called the Bellman equation. Equation (103) is equivalent to the following two equations

$$\frac{\partial F}{\partial \dot{x}_i} + \frac{\partial S}{\partial x_i} = 0, \qquad i = 1, 2, \ldots, s \quad (104)$$

which is obtained by taking the derivative of Equation (103) with respect to $\dot{x}_i$ and

$$F + \frac{\partial S}{\partial t} + \sum_{i=1}^{s} \dot{x}_i \frac{\partial S}{\partial x_i} = 0 \, , \quad (105)$$

which is the minimum value of Equation (101). Differentiating Equation (104) with respect to t gives

$$\frac{d}{dt} \frac{\partial F}{\partial \dot{x}} + \frac{\partial^2 S}{\partial x_i \, \partial t} + \sum_{j=1}^{s} \frac{\partial^2 S}{\partial x_i \, \partial x_j} \dot{x}_j = 0 \, , \qquad i = 1, 2, \ldots, s. \quad (106)$$

Partial differentiation of Equation (105) with respect to $x_i(t)$ yields

$$\frac{\partial F}{\partial x_i} + \sum_{j=1}^{s} \frac{\partial F}{\partial \dot{x}_j} \frac{\partial \dot{x}_j}{\partial x_i} + \frac{\partial^2 S}{\partial t \, \partial x_i} + \sum_{j=1}^{s} \dot{x}_j \frac{\partial^2 S}{\partial x_j \, \partial x_i} + \sum_{j=1}^{s} \frac{\partial S}{\partial x_j} \frac{\partial \dot{x}_j}{\partial x_i} = 0 \, ,$$

$$i = 1, 2, \ldots, s$$

which may be reduced to

$$\frac{\partial F}{\partial x_i} + \frac{\partial^2 S}{\partial t \, \partial x_i} + \sum_{j=1}^{s} \dot{x}_j \frac{\partial^2 S}{\partial x_j \, \partial x_i} = 0 \, , \qquad i = 1, 2, \ldots, s \quad (107)$$

by using Equation (104). Substracting Equation (104) from Equation (107) gives the set of Euler-Lagrange equations

$$\frac{\partial F}{\partial x_i} - \frac{d}{dt}\frac{\partial F}{\partial \dot{x}_i} = 0 , \qquad i = 1, 2, \ldots, s. \tag{108}$$

In deriving Equation (104) the fact that the first derivative must be zero at a minimum point was used. Meanwhile, at the minimum point the second derivative must be

$$\frac{\partial^2 F}{\partial \dot{x}_i \, \partial \dot{x}_j} \geq 0 , \tag{109}$$

which is the Legendre necessary condition for a minimum.

It follows from Equation (103) that for the optimal decision $\bar{\dot{x}}(t)$ (or $\bar{\theta}(t)$) one has the following inequality

$$F(t, x(t), \theta(t)) + \frac{\partial S}{\partial t} + \sum_{i=1}^{s} \frac{\partial S}{\partial x_i} \theta_i(t) \geq$$

$$F(t, x(t), \bar{\theta}(t)) + \frac{\partial S}{\partial t} + \sum_{i=1}^{s} \frac{\partial S}{\partial x_i} \bar{\theta}_i(t) \quad ,$$

or

$$F(t, x(t), \theta(t)) - F(t, x(t), \bar{\theta}(t)) + \sum_{i=1}^{s} (\theta_i(t) - \bar{\theta}_i(t)) \frac{\partial S}{\partial x_i} \geq 0. \tag{110}$$

Because of Equation (104), Equation (110) becomes

$$F(t, x(t), \theta(t)) - F(t, x(t), \bar{\theta}(t)) - \sum_{i=1}^{s} (\theta_i(t) - \bar{\theta}_i(t)) \frac{\partial F}{\partial \bar{\theta}_i} \geq 0. \tag{111}$$

This is the Weierstrass necessary condition for a minimum. Now consider that the final point of the trajectory lies on the curve

$$x = g(T). \tag{112}$$

Then for the optimal curve, the change in S as the final point varies along the given curve must be zero, that is

$$\frac{\partial S}{\partial t} + \sum_{i=1}^{s} \frac{\partial S}{\partial x_i} \frac{dg_i}{dt} = 0 , \tag{113}$$

at $t = \bar{T}$. Combining Equations (104), (105), and (113), one obtains

$$F + \sum_{i=1}^{s} \left(\frac{dg_i}{dt} - \dot{x}_i\right) \frac{\partial F}{\partial \dot{x}_i} = 0 \ , \tag{114}$$

which is equivalent to Equation (70), the transversality condition at the final point.

The relationships among the maximum principle, dynamic programming, and the calculus of variations have been discussed. It is recognized that there is no single optimization technique superior to other techniques in handling every type of problems. How to choose an appropriate technique to solve a specific type of problem is an important step. The selection of a proper technique depends on the characteristics of the problem, the computing facilities, such as analog or digital computers, and other factors influencing the calculations in the problem.

The Maximum Principle and the Adjoint System

There are several ways of deriving the algorithms. The derivations using adjoint systems and Green's functions (23, 24) will be discussed. A numerical iterative technique which uses the Green's function will also be briefly described.

Without loss of generality, one can consider the autonomous system

$$\frac{dx_i}{dt} = \dot{x}_i = f_i(x(t),\ \theta(t)) \ , \qquad i = 1,\ 2, \ldots,\ s \tag{113}$$

and an objective function of the form

$$S = \sum_{i=1}^{s} c_i \ x_i(T).$$

Let $(\bar{x}(t);\ \bar{\theta}(t))$ be the optimal point. Then the variational equations are

$$x(t) = \bar{x}(t) + \delta x(t) , \tag{114}^*$$

$$\theta(t) = \bar{\theta}(t) + \delta\theta(t). \tag{115}^*$$

Considering the variations of f_i both in x_i and θ_i simultaneously and linearizing yields

$$\delta\dot{x}_i = \sum_{j=1}^{s} \frac{\partial f_i}{\partial x_j} \delta x_j + \sum_{k=1}^{r} \frac{\partial f_i}{\partial \theta_k} \delta\theta_k , \qquad i = 1, 2, \ldots, s. \tag{116}$$

The partial derivatives are evaluated along the optimal path. For the fixed initial point,

$$\delta x_i(t_0) = 0, \qquad i = 1, 2, \ldots, s.$$

The so-called adjoint system of Equation (116) is defined by

$$\frac{dz_i}{dt} = \dot{z}_i(t) = - \sum_{j=1}^{s} \frac{\partial f_j}{\partial x_i} z_j , \qquad i = 1, 2, \ldots, s. \tag{117}$$

It is obtained by deleting the control terms and transposing the matrix of coefficients and changing the sign. The adjoint vector $z(t)$ may also be called Green's vector.

Substituting Equations (116) and (117) into the following equation,

$$\frac{d}{dt} \sum_{i=1}^{s} z_i \, \delta x_i = \sum_{i=1}^{s} \dot{z}_i \, \delta x_i + \sum_{i=1}^{s} z_i \, \delta\dot{x}_i ,$$

gives

$$\frac{d}{dt} \sum_{i=1}^{s} z_i \, \delta x_i = \sum_{i=1}^{s} \sum_{j=1}^{r} z_i \frac{\partial f_i}{\partial \theta_j} \delta\theta_j . \tag{118}$$

Equation (118) is equivalent to Equation (14) of Section II. Integrating Equation (118) from $t = t_0$ to $t = T$, one obtains

$$\sum_{i=1}^{s} \left[z_i(T) \, \delta x_i(T) - z_i(t_0) \, \delta x_i(t_0) \right] = \int_{t_0}^{T} \sum_{i=1}^{s} \sum_{j=1}^{r} z_i \frac{\partial f_i}{\partial \theta_j} \delta\theta_j \, dt. \tag{119}$$

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* Equations (114) and (115) are the same as used previously. Here $\delta x(t)$ includes the terms ϵy and $O(\epsilon^2)$ and $\delta\theta(t)$ includes $\epsilon\varphi$ and $O(\epsilon^2)$.

Suppose that the boundary conditions of z_i are defined as

$$z_i(T) = c_i \,, \qquad i = 1, 2, \ldots, s.$$

Since

$$\delta x_i(t_0) = 0, \qquad i = 1, 2, \ldots, s$$

and the variation of the objective function is zero along the optimal trajectory, that is

$$\delta S = \sum_{i=1}^{s} c_i \, \delta x_i(T) = 0 \,. \tag{120}$$

Equation (119) therefore becomes

$$\sum_{i=1}^{s} c_i \, \delta x_i(T) = \int_{t_0}^{T} \sum_{i=1}^{s} \sum_{j=1}^{r} z_i \frac{\partial f_i}{\partial \theta_j} \delta\theta_j \, dt = 0 \,, \tag{121}$$

or

$$\sum_{i=1}^{s} z_i \frac{\partial f_i}{\partial \theta_j} = \frac{\partial H}{\partial \theta_j} = 0 \,, \qquad j = 1, 2, \ldots, r.$$

This is the necessary condition for the weak form of the maximum principle (18) (the difference between the weak and strong forms of the maximum principle will be discussed later).

It has been shown that it is also convenient to use Green's functions (see Appendix 2) to derive the above conditions (23, 24, 25).

A solution of Equation (116) may be written in the form

$$\delta x_i(t) = \sum_{j=1}^{s} G_{ij}(t_0, t) \, \delta x_j(t_0) + \int_0^t \sum_{j=1}^{s} G_{ij}(t, \tau) \sum_{k=1}^{r} \frac{\partial f_j}{\partial \theta_k} \delta\theta_k \, d\tau \tag{122}$$

where $G_{ij}(t, \tau)$ are called Green's functions (or influence functions). The first term on the right hand side of Equation (122) represents solutions of the homogeneous system of equations. Green's functions transmit the influence of a unit impulse (or Dirac delta function) in the decision variables at

time τ, or unit change in $x_i(0)$, to the output $x_i(t)$.

Multiplying both sides of Equation (122) by $z_i(T)$ and summing

$$\sum_{i=1}^{s} z_i(T)\ \delta x_i(T) = \sum_{j=1}^{s} z_j(t_0)\ \delta x_j(t_0) + \int_{t_0}^{T} \sum_{j=1}^{s} z_j(t) \sum_{k=1}^{r} \frac{\partial f_j}{\partial \theta_k} \delta\theta_k\, d\tau$$

$$= \sum_{i=1}^{s} z_i(t_0)\ \delta x_i(t_0) + \int_{t_0}^{T} \sum_{i=1}^{s} \sum_{j=1}^{r} z_i \frac{\partial f_i}{\partial \theta_j} \delta\theta_j\, d\tau \tag{123}$$

which is the same as Equation (119) and equivalent to Equation (15) of Section II. This is also called Green's Identity.

Whenever the variational equation, Equation (116) is written, a formal solution, Equation (122), can be obtained by using Green's functions. Green's Identity, Equation (123), follows immediately by taking the inner product.

Green's functions also lead to computational schemes for the solution of optimization problems. Solving optimization problems by means of the maximum principle results in two point boundary value problems. Usually we have problems in which the initial conditions are given for the system equations and the final conditions are given for the adjoint system of equations (or adjoint systems). An iterative technique must be used to treat these problems.

Assume that $\theta(t)$ lies in the δ-neighborhood of $\bar{\theta}(t)$, $\delta\theta(t)$ must be assumed to be approximately zero. Equation (122), then, is approximated by

$$\delta x_i(T) = \sum_{j=1}^{s} G_{ij}(t_0,t)\ \delta x_j(t_0). \tag{124}$$

Let $x'(T)$ be the guessed final value of the state vector. If it corresponds to an initial value $x'(t_0)$, instead of the given initial value $x(t_0)$, one can obtain a better guess of $x(T)$ by using the following iterative equation

obtained from Equation (124)

$$x_i(T) = x_i'(T) + \sum_{j=1}^{s} G_{ij}(t_0, t) \left[x_j(t_0) - x_j'(t_0)\right]. \tag{125}$$

This scheme is based on the work of Bliss (26) and Goodman and Lance (27). Denn and Aris first applied it to the problem of optimization (24). Green's functions can also be associated with the method of gradients (or method of steepest descent) to solve the optimization problems computationally (23, 28, 29).

The Weak and Strong Forms of the Maximum Principle

Algorithms have been derived for the weak form of the maximum principle for both the simple and complex discrete (6) as well as continuous systems by using the first order variational equations. When the objective function is to be maximized (or minimized), the Hamiltonian function is made stationary with respect to the optimal decisions which lie in the interior of an admissible region, and H is made minimum (or maximum) when they lie at the boundary of the admissible region.

It has been pointed out that there is no exact analogue of the discrete maximum principle to the continuous one. In the discrete system it is shown that there exists only the weak form of the maximum principle (30, 31, 32, 33).

The algorithm for the strong maximum principle can be obtained by considering the second order terms in the variational equations (31, 32, 33). In the following the strong form of the maximum principle is obtained for simple continuous systems. Taking into account the second order terms, Equation (11) of Section II can be written as

$$\epsilon \frac{dy_i}{dt} = f_i(x;\, \theta) - f_i(\bar{x};\, \bar{\theta}) + O(\epsilon^2)$$

$$= \sum_j \frac{\partial f_i}{\partial x_j} \epsilon y_j + \frac{1}{2} \sum_{j,k} \frac{\partial^2 f_i}{\partial x_j \, \partial x_k} (\epsilon y_j)(\epsilon y_k) + \frac{1}{2} \sum_{j,k} \frac{\partial^2 f_i}{\partial x_j \, \partial \theta_k} (\epsilon y_j)(\epsilon \varphi_k)$$

$$+ \sum_j \frac{\partial f_i}{\partial \theta_j} \epsilon \varphi_j + \frac{1}{2} \sum_{j,k} \frac{\partial^2 f_i}{\partial \theta_j \, \partial \theta_k} (\epsilon \varphi_j)(\epsilon \varphi_k) + 0(\epsilon^3), \quad t_0 \le t \le T$$

$$i = 1, 2, \ldots, s \qquad (126)^*$$

where the partial derivatives are evaluated along the optimal trajectory and $0(\epsilon^3)$ represents the terms of order ϵ^3 and those of order higher than ϵ^3 such that

$$\lim_{\epsilon \to 0} \frac{0(\epsilon^3)}{\epsilon^2} = 0.$$

Using Green's functions, one obtains a solution for Equation (126) as

$$\epsilon y_i(t) = \sum_j G_{ij}(t_0, t) \, \epsilon y_j(t_0) + \int_{t_0}^{t} \sum_{j,k} G_{ij}(t,\tau) \frac{\partial f_j}{\partial \theta_k} \epsilon \varphi_k \, d\tau$$

$$+ \frac{1}{2} \int_{t_0}^{t} \sum_{j,k,m} G_{ij}(t,\tau) \frac{\partial^2 f_j}{\partial \theta_k \, \partial \theta_m} (\epsilon \varphi_k)(\epsilon \varphi_m) \, d\tau$$

$$+ \frac{1}{2} \int_{t_0}^{t} \sum_{j,k,m} G_{ij}(t,\tau) \frac{\partial^2 f_j}{\partial x_k \, \partial \theta_m} (\epsilon y_k)(\epsilon \varphi_m) \, d\tau$$

$$+ \frac{1}{2} \int_{t_0}^{t} \sum_{j,k,m} G_{ij}(t,\tau) \frac{\partial^2 f_j}{\partial x_k \, \partial x_m} (\epsilon y_k)(\epsilon y_m) + 0(\epsilon^3) \, ,$$

$$t_0 \le t \le T; \qquad i = 1, 2, \ldots, s. \qquad (127)$$

Successive approximation by substituting $\epsilon y(t)$ into Equation (127) itself gives

$$\epsilon y_i(T) = \sum_j G_{ij}(t_0, T) \, \epsilon y_j(t_0) + \int_{t_0}^{T} \sum_{j,k} G_{ij}(T,\tau) \frac{\partial f_j}{\partial \theta_k} \epsilon \varphi_k \, d\tau$$

---

* $\sum_{j,k}$ denotes the summation over the j and k subscripts. j and k range from one to s for x and one to r for θ.

$$+ \frac{1}{2} \int_{t_0}^{T} \sum_{j,k,m} G_{ij}(t,\tau) \frac{\partial^2 f_j}{\partial\theta_k\, \partial\theta_m} (\epsilon\varphi_k)(\epsilon\varphi_m)\, d\tau$$

$$+ \frac{1}{2} \int_{t_0}^{T} \sum_{j,k,m} G_{ij}(T,\tau) \frac{\partial^2 f_j}{\partial x_k\, \partial\theta_m} \epsilon\varphi_m \left\lfloor \int_{t_0}^{T} \sum_{j,m} G_{kj} \frac{\partial f_j}{\partial\theta_m} \epsilon\varphi_m\, dt \right\rfloor d\tau$$

$$+ \frac{1}{2} \int_{t_0}^{T} \sum_{j,k,m} G_{ij}(T,\tau) \frac{\partial^2 f_j}{\partial x_k\, \partial x_m} \left\lfloor \int_{t_0}^{T} \sum_{j,m} G_{kj} \frac{\partial f_j}{\partial\theta_m} \epsilon\varphi_m\, dt \right\rfloor d\tau$$

$$+ \left\lfloor \int_{t_0}^{T} \sum_{j,k} G_{mj} \frac{\partial f_j}{\partial\theta_k} \epsilon\varphi_k\, dt \right\rfloor d\tau + 0(\epsilon^3) \qquad (128)$$

$$i = 1, 2, \ldots, s, \qquad t_0 \leq t \leq T.$$

Now consider the special variations (30, 33)

$$\epsilon\varphi(t) = \begin{cases} \epsilon\bar{\varphi}(t)\,, & t_1 \leq t \leq t_1 + \Delta t \\ 0\,, & \text{otherwise.} \end{cases} \qquad (129)$$

If the initial state is assumed to be fixed, that is

$$\epsilon y(t_0) = 0\ ,$$

the first two terms on the right hand side of Equation (128) are of the order Δt and the remaining terms are of the order $(\Delta t)^2$ and of order higher than $(\Delta t)^2$. Letting Δt be sufficiently small, one obtains

$$\epsilon y_i(T) = \int_{t_1}^{t_1+\Delta t} \sum_{j,k} G_{ij}(T,\tau) \frac{\partial f_j}{\partial\theta_k} \epsilon\bar{\varphi}_k\, d\tau$$

$$+ \frac{1}{2} \int_{t_1}^{t_1+\Delta t} \sum_{j,k,m} G_{ij}(T,\,\tau) \frac{\partial^2 f_j}{\partial\theta_k\, \partial\theta_m} (\epsilon\bar{\varphi}_k)(\epsilon\bar{\varphi}_m)\, d\tau$$

$$+ 0(\epsilon^3) + 0\left\lfloor (\Delta t)^2 \right\rfloor . \qquad (130)$$

where $0(\Delta t)^2$ represents second and higher order terms. The objective function is of the form

$$S = \sum_i c_i x_i(T), \qquad i = 1, 2, \ldots, s$$

where

$$z_i(T) = c_i \ , \qquad i = 1, 2, \ldots, s.$$

As in Equation (123), taking the inner product of Equation (130) and z(T) yields

$$\sum_i \epsilon y_i(T)\, c_i = \int_{t_1}^{t_1+\Delta t} \sum_{j,k} z_j(t) \frac{\partial f_j}{\partial \theta_k} \epsilon\bar{\varphi}_k \, d\tau$$

$$+ \frac{1}{2} \int_{t_1}^{t_1+\Delta t} \sum_{j,k,m} z_j(t) \frac{\partial^2 f_j}{\partial \theta_k \, \partial \theta_m} (\epsilon\bar{\varphi}_k)(\epsilon\bar{\varphi}_m) \, d\tau$$

$$+ 0(\epsilon^3) + 0\left[(\Delta t)^2\right]$$

$$= \int_{t_1}^{t_1+\Delta t} \sum_k \frac{\partial H}{\partial \theta_k} \epsilon\bar{\varphi}_k \, d\tau$$

$$+ \frac{1}{2} \int_{t_1}^{t_1+\Delta t} \sum_{k,m} \frac{\partial^2 H}{\partial \theta_k \, \partial \theta_m} (\epsilon\bar{\varphi}_k)(\epsilon\bar{\varphi}_m) \, d\tau$$

$$+ 0(\epsilon^3) + 0\left[(\Delta t)^2\right] . \qquad (131)$$

For the objective function to be a maximum, one has

$$\sum_i \epsilon y_i(T)\, c_i < 0 \ . \qquad (132)$$

The weak form of the maximum principle requires that

$$\frac{\partial H}{\partial \theta_k} = 0 \ , \qquad k = 1, 2, \ldots, r \ , \qquad t_1 \leq t \leq t_1 + \Delta t. \qquad (133)$$

Therefore,

$$\int_{t_1}^{t_1+\Delta t} \sum_{k,m} \frac{\partial^2 H}{\partial \theta_k \, \partial \theta_m} (\epsilon\bar{\varphi}_k)(\epsilon\bar{\varphi}_m) \, d\tau < 0 \ . \qquad (134)$$

Since t_1 and $\epsilon\bar{\varphi}$ are arbitrary, and Δt may be chosen as small as one desires, the Hessian matrix whose kmth element is

$$\frac{\partial^2 H}{\partial \theta_k \, \partial \theta_m}$$

must be positive definite at all but a finite number of points (30, 31, 32). Hence it is concluded that in maximizing (minimizing) an objective function, the Hamiltonian function must be a maximum (or minimum) at all but a finite number of points. If the Hessian matrix is semipositive definite one can obtain the same result by considering higher order terms. The above derivations using tensor and matrix notation were obtained by Jackson and Horn (31, 32) and Denn and Aris (33).

The basic difference between the continuous and discrete cases, as Polak, Jackson, and Horn have noticed, is that in the former one can use a sufficiently small interval of time Δt to simplify the result while in the latter no small interval of Δt can be adjusted. The strong maximum principle for different cases was considered by Jackson, Horn, Denn and Aris (30, 31, 32). So far as applications to the solution of problems are concerned, both the strong and weak forms of the maximum principle lead to the same result for continuous processes.

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APPENDICES

APPENDIX I

Pontryagin's maximum principle (10) can be summarized in the following theorem:

Let $\theta(t)$, $t_0 \leq t \leq T$ be a piecewise continuous vector function satisfying the constraints given by

$$\psi_i \left[\theta_1(t),\ \theta_2(t), \ldots,\ \theta_r(t)\right] < 0\ , \qquad i = 1,\ 2, \ldots,\ m.$$

In order that the objective function S be a maximum (or minimum), it is necessary that there exist a nonzero continuous vector $z(t)$ satisfying

$$\frac{dz_i}{dt} = -\frac{\partial H}{\partial x_i}\ , \qquad i = 1,\ 2, \ldots,\ s \tag{1}$$

$$z_i(T) = c_i\ , \qquad i = 1,\ 2, \ldots,\ s \tag{2}$$

and that the vector function $\theta(t)$ be chosen that $H(z,x,\theta)$, is a maximum (or minimum) for every t, $t_0 \leq t \leq T$. Furthermore, the maximum (or minimum) value of H is constant for every t.

Based on this theorem it can be shown that

$$\max \text{ (or min) } H = 0\ ,$$

if the time interval is not fixed. Assume that $\bar{x}(t)$ and $\bar{\theta}(t)$ are the optimal trajectory and decision, and let $\bar{T}$ be the final time corresponding to them. Then the problem may now be considered as a fixed time problem with the final time fixed at $\bar{T}$ and with the initial given conditions. Therefore, the objective function S defined for a fixed time problem becomes

$$S = \sum_{i=1}^{s} c_i x_i(\bar{T}). \tag{3}$$

and correspondingly the components of the adjoint vector take the value of c_i at $t = \bar{T}$, that is

$$z_i(\bar{T}) = c_i \;, \qquad i = 1, 2, \ldots, s. \tag{4}$$

Consider now a variation of the objective function S resulting from a very small change of time, from $\bar{T}$ to $\bar{T} + \delta T$, along the optimal trajectory $\bar{x}(t)$. One has

$$\begin{aligned}
\delta S &= \sum_{i=1}^{s} c_i \, \bar{x}_i(\bar{T} + \delta T) - c_i \, \bar{x}_i(\bar{T}) \\
&= \sum_{i=1}^{s} c_i \frac{d\bar{x}_i}{dt} \Bigg|_{t=\bar{T}} \delta T = \sum_{i=1}^{s} z_i(\bar{T}) \frac{d\bar{x}_i}{dt} \Bigg|_{t=\bar{T}} \delta T \\
&= H \Bigg|_{t=\bar{T}} \delta T \,.
\end{aligned} \tag{5}$$

Since δS must be greater than or equal to zero for a minimum of S (or δS must be less than or equal to zero for a maximum of S) and δT may be positive or negative, one may conclude that

$$\delta S = 0 \;,$$

that is

$$H \Bigg|_{t=\bar{T}} = 0.$$

From the above theorem it is known that the extremum of H is constant for every t, $t_0 \leq t \leq \bar{T}$. It follows that

$$\min H = 0 \quad \text{for} \quad 0 \leq t \leq \bar{T}.$$

APPENDIX II

Consider the system of the non-homogeneous linear differential equations

$$L(x) = p_0 \frac{d^n x_i}{dt^n} + p_1 \frac{d^{n-1} x_i}{dt^{n-1}} + \dots + p_n x_i = r_i(t), \tag{8}$$

$$i = 1, 2, \dots, s.$$

$$u_j(x) = \gamma_j , \qquad j = 1, 2, \dots, s. \tag{9}$$

There exists a Green's function $G_{ij}(t,\tau)$ such that (34)

a) the solution of Equation (8) can be written as

$$x_i(t) = \sum_{j=1}^{s} G_{ij}(t_0,t)\, \gamma_j + \int_{t_0}^{t} \sum_{j=1}^{s} G_{ij}(t,\tau)\, \gamma_i(\tau)\, d\tau \tag{10}$$

$$i = 1, 2, \dots, s$$

b) $G_{ij}(t,\tau)$ is continuous and possesses continuous derivatives of orders up to and including (n-2) when $t_0 \leq t \leq T$

c) the derivative of order (n-1) is discontinuous at a point τ within (t_0,T), the discontinuity being an upward jump of amount $1/p_0(\tau)$

d) $G_{ij}(t,\tau)$ satisfies the differential equation at all points of (t_0,τ) except τ.

For the variational equations of the performance equations

$$\delta\dot{x}_i = \sum_{j=1}^{s} \frac{\partial f_i}{\partial x_j}\, \delta x_j + \sum_{k=1}^{r} \frac{\partial f_i}{\partial \theta_k}\, \delta\theta_k , \quad i = 1, 2, \dots, s \tag{4.116}$$

by using Green's function the solution may be written as

$$\delta x_i(t) = \sum_{j=1}^{s} G_{ij}(t_0,t)\, \delta x_j(t_0) + \int_{t_0}^{t} \sum_{k=1}^{s} G_{ij}(t,\tau) \sum_{k=1}^{r} \frac{\partial f_j}{\partial \theta_k}\, \delta\theta_k\, d\tau. \tag{11}$$

In order to relate the Green's function to the adjoint vector z(t), one

defines the following:

$$z_{ij}(T) = \delta_{ij} ,$$
$$G_{ij}(T, t) = z_{ij}(t), \tag{12}$$
$$G_{ij}(t_0, T) = z_{ij}(t_0).$$

Since

$$z_i(T) = c_i , \qquad i = 1, 2, \ldots, s \tag{2.6}$$

or

$$z_i(T) = c_i = \sum_{j=1}^{s} c_j \, \delta_{ji} = \sum_{j=1}^{s} c_j \, z_{ji}(T). \tag{13}$$

Thus Equation (11) becomes

$$\delta x_i(T) = \sum_{j=1}^{s} z_{ij}(t_0) \, \delta x_j(t_0) + \int_{t_0}^{T} \sum_{j=1}^{s} z_{ij}(t) \sum_{k=1}^{r} \frac{\partial f_j}{\partial \theta_k} \, \delta\theta_k \, d\tau. \tag{14}$$

From the linearity and homogeneity of the adjoint system, it can be concluded that

$$z_i(t) = \sum_{j=1}^{s} c_i \, z_{ji}(t) \qquad \text{for} \qquad t_0 \leq t \leq T. \tag{15}$$

The inner product of a constant vector with z_{ij} gives the adjoint vector, z.

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NOMENCLATURE

a	vector belonging to a tangent plane
b	number of initial points
c	number of continuous branches
c'	number of entering streams which are continuous
c"	number of leaving streams which are continuous
c_i	constant in objective function
d	number of discrete branches
d'	number of entering streams which are discrete
d"	number of leaving streams which are discrete
E	Weierstrass excess function
f_i	real function
F	real function
g	real function
G_{ij}	Green's function
h	real function
H	Hamiltonian function
k	kth branch
m	mth stage
M	constant
n	nth stage
N	total number of branches or total number of discrete stages or the Nth discrete stage
P	profit function
r	dimension of the decision vector
R	region of the space of real variables

s	dimension of the state vector
S	objective function
t	time
t_0	initial value of time t
t'	time as a dummy variable
T	final value of time
W	real function
x	state vector
$\bar{x}$	optimal state vector
$\dot{x}$	derivative of x with respect to t
y	perturbation of the state vector
z	adjoint vector or Green's vector
z_{ij}	Green's tensor

Greek Letters

α	constant
β	constant
δ_{ij}	Kronecker delta
ϵ	small number
η	parameter
γ	constant
θ	decision vector
$\bar{\theta}$	optimal decision vector
ξ	constant
τ	parameter
λ	constant

μ constant

φ perturbation of the decision vector

ψ real function

OPTIMIZATION OF COMPOSITE PROCESSES
AND VARIATIONAL TECHNIQUES

by

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The main purpose of this work is to develop the working algorithms for the optimization of a topologically composite processes by applying the maximum principle.

The basic algorithms of the maximum principle for simple continuous and discrete processes are first presented. A composite process is composed of both complex continuous and discrete processes. The algorithms derived are applicable to such a process without decomposing the process into simple subprocesses. To illustrate the use of the algorithms, two examples are solved.

The underlying idea of the maximum principle is closely related to other variational techniques. The relationships between the calculus of variations and the maximum principle are discussed. The main advantage of the latter over the former is that it can be used to solve problems in which the decision variables are constrained. These problems can not be solved using the calculus of variations. For the unconstrained case, the basic algorithms of the maximum principle are shown to be equivalent to the Euler-Lagrange equation and they conform to the Weierstrass necessary condition. The transformation used in the maximum principle is essentially the same as the canonical transformation in the calculus of variations. The basic algorithms of the maximum principle and those of dynamic programming are compared. Finally, the weak and strong forms of the maximum principle, which have been strongly argued recently are presented. It is concluded that there is no exact analog of the continuous maximum principle for the discrete maximum principle. The discrete maximum principle uses only a weak condition, that is, when the objective function has a maximum (or minimum) the Hamiltonian function attains a stationary value. The continuous

maximum principle has a strong condition, that is, if the objective function has a maximum (or minimum), then the Hamiltonian function attains its maximum (or minimum) value.